Scientific Computing with Amazon Web Services

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http://bit.ly/AWSOSG



Amazon Global Impact Initiatives

Scientific Computing

- Global "Big Science" Projects
- Enabling the "long tail of science"
- Collaborative research
- Accelerating the transition to "Networked Science"

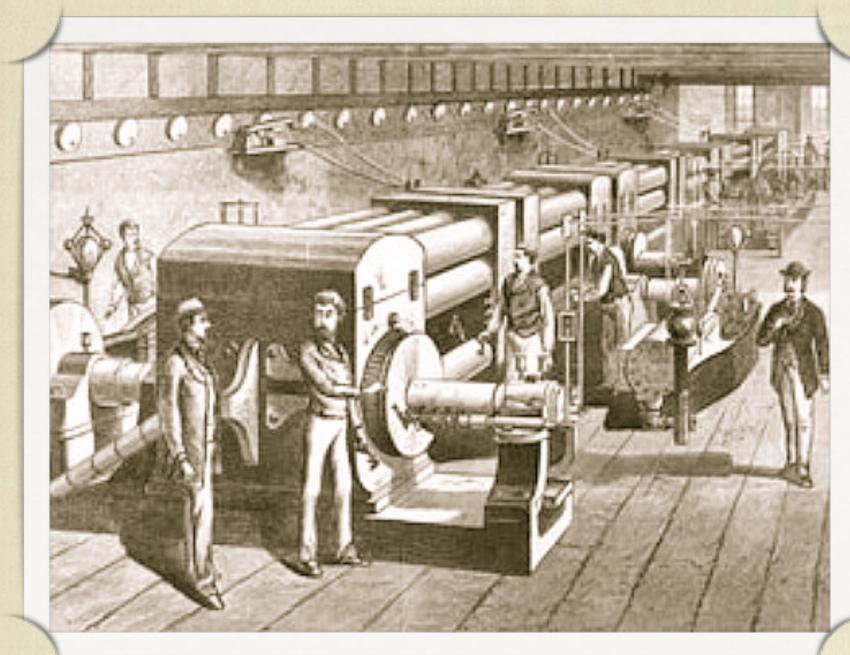
- AWS as the platform for open-access data portals and archives
- Amazon Public Data Sets
- Public/Private Data partnerships

Eaconomic Development

- The Amazon Job Accelerators program

Why are we focusing on the Scientific Community?

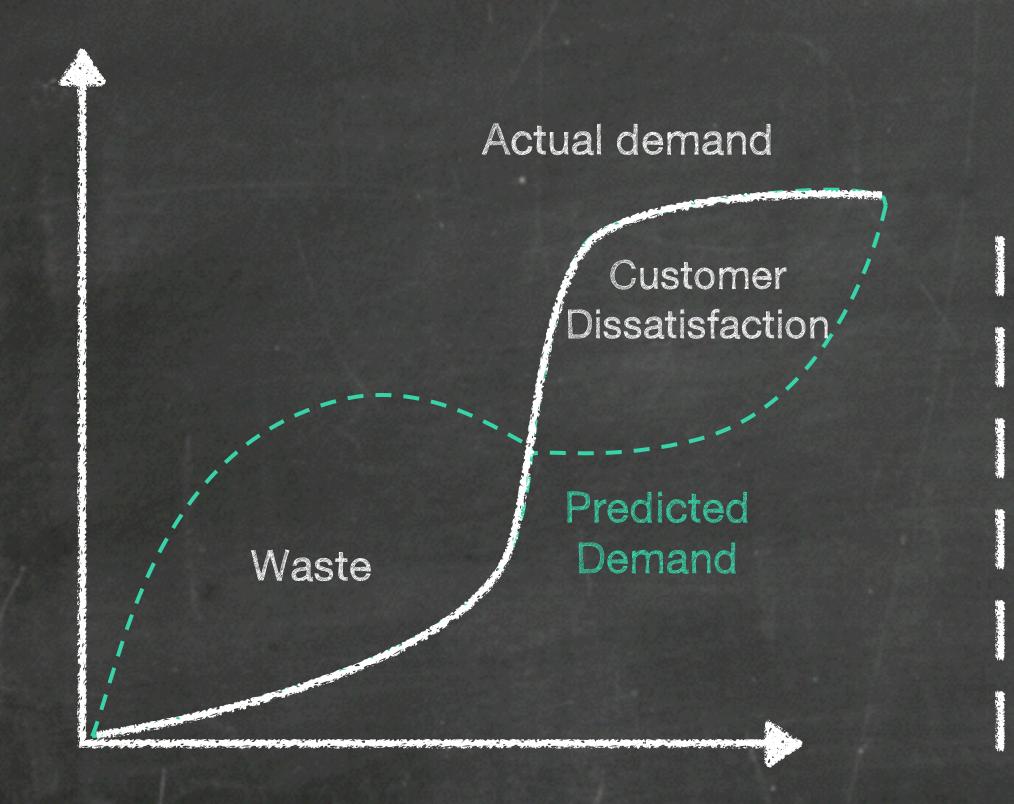
- o Scientific computing is a profitable business for AWS
- To accelerate the pace of scientific discovery
- To develop new capabilities which will benefit all AMS customers
 - Streaming data processing & analytics
 - Exabyte scale data management solutions
 - Collaborative research tools and techniques
 - New AWS regions (e.g. South Africa and Western Australia for the SKA)
 - Significant advances in low-power compute, storage and data centers
 - Identify efficiencies which will lower our costs and pricing for customers
 - Push our existing services to support exabyte/exaflop scale workloads



Pearl Street Power Station



SOF HOSTING







amazon.com

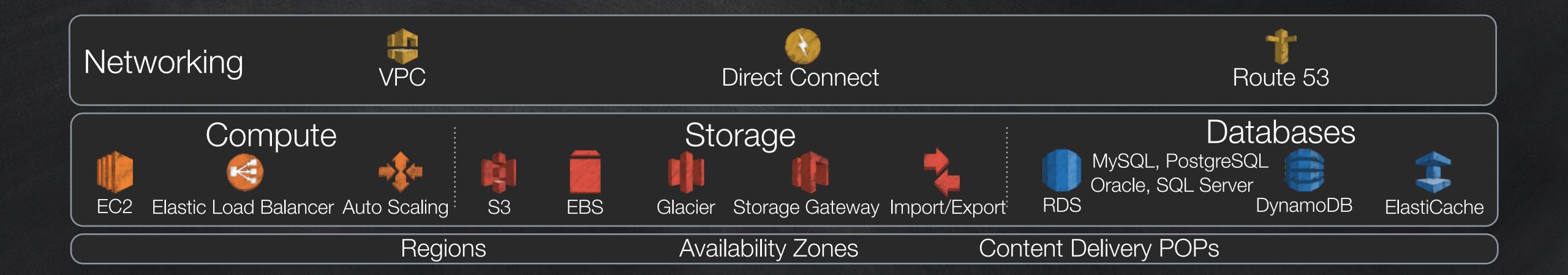
\$5.2B retail business
7,800 employees
A whole lot of servers

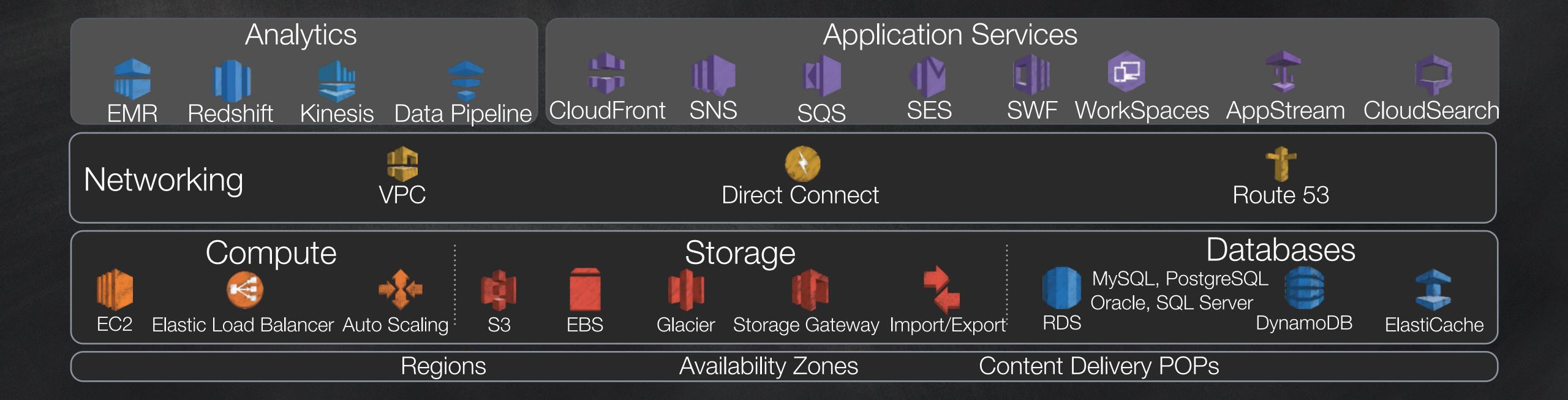


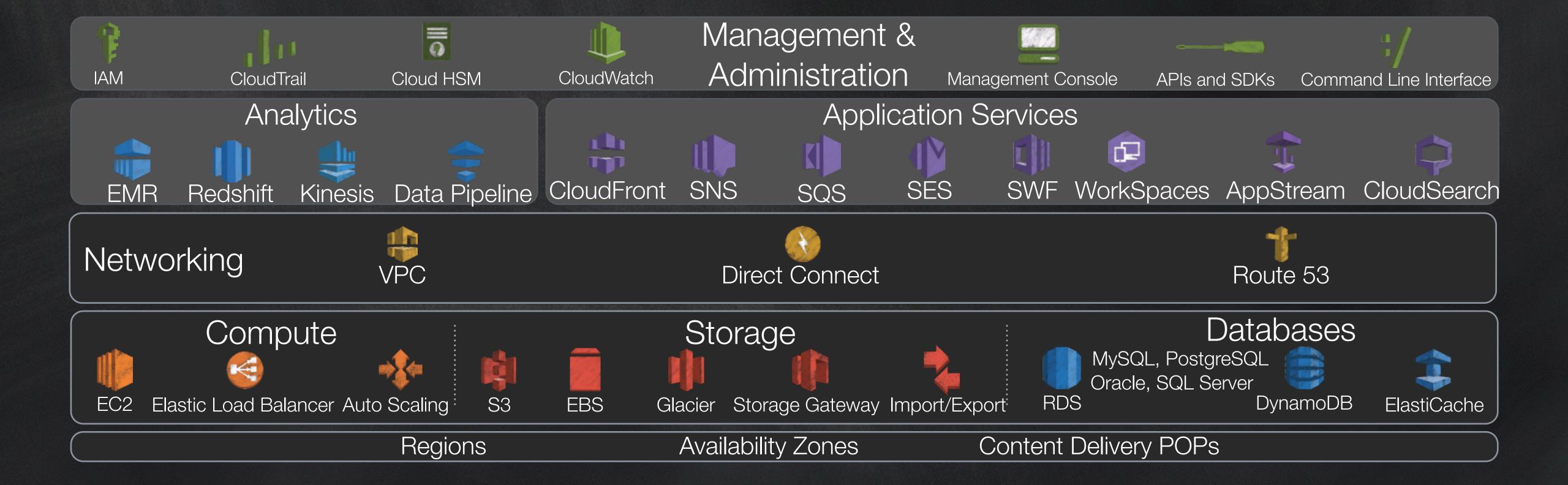
Every day, AWS adds enough server capacity to power this \$5B enterprise

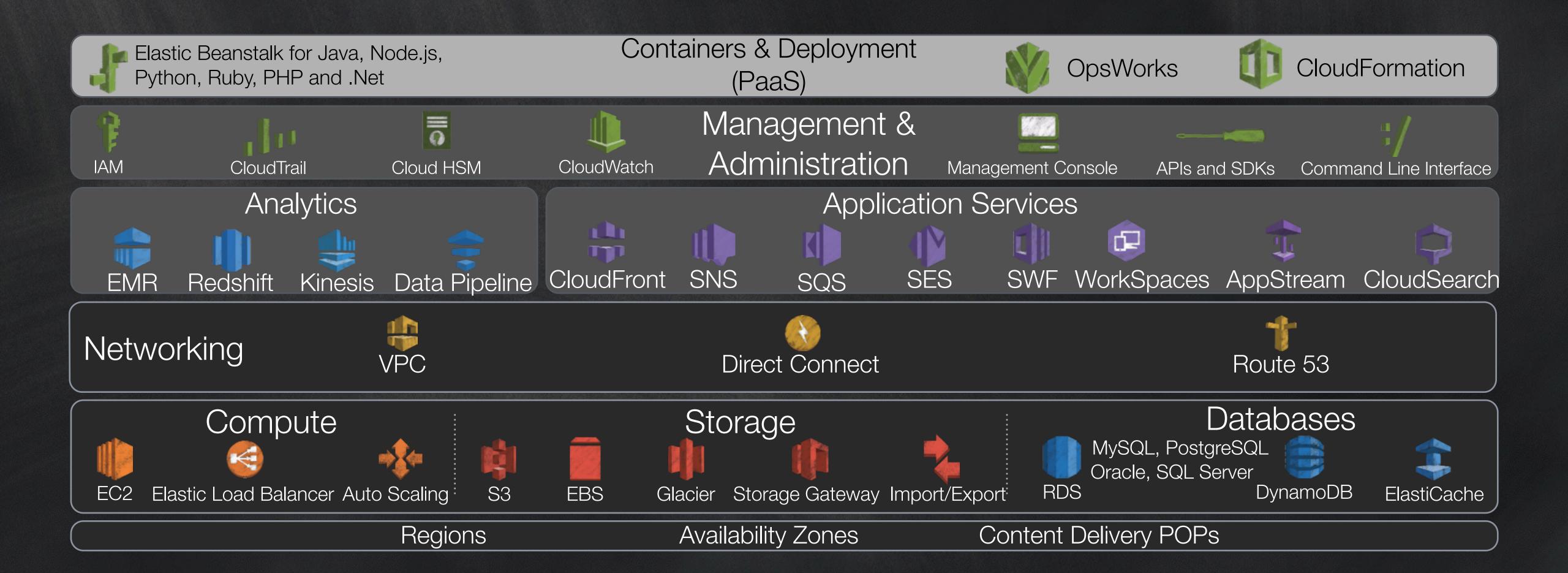


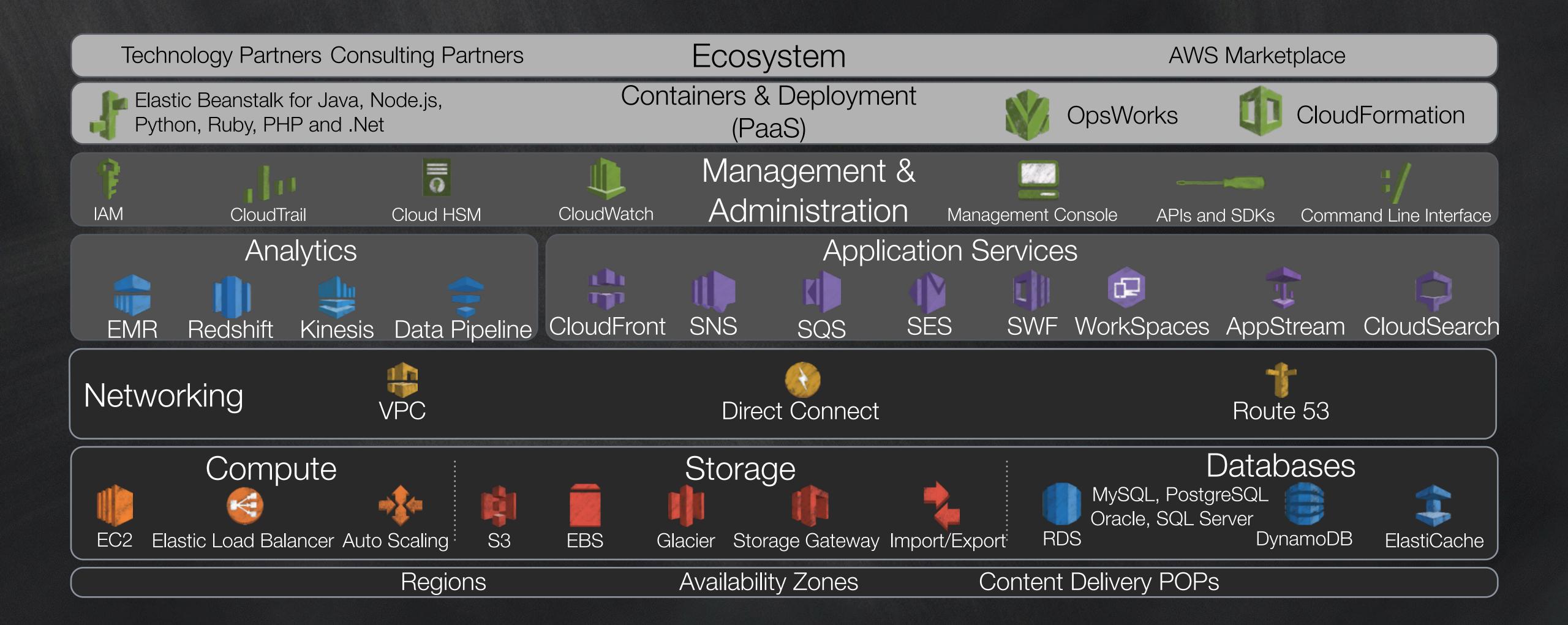


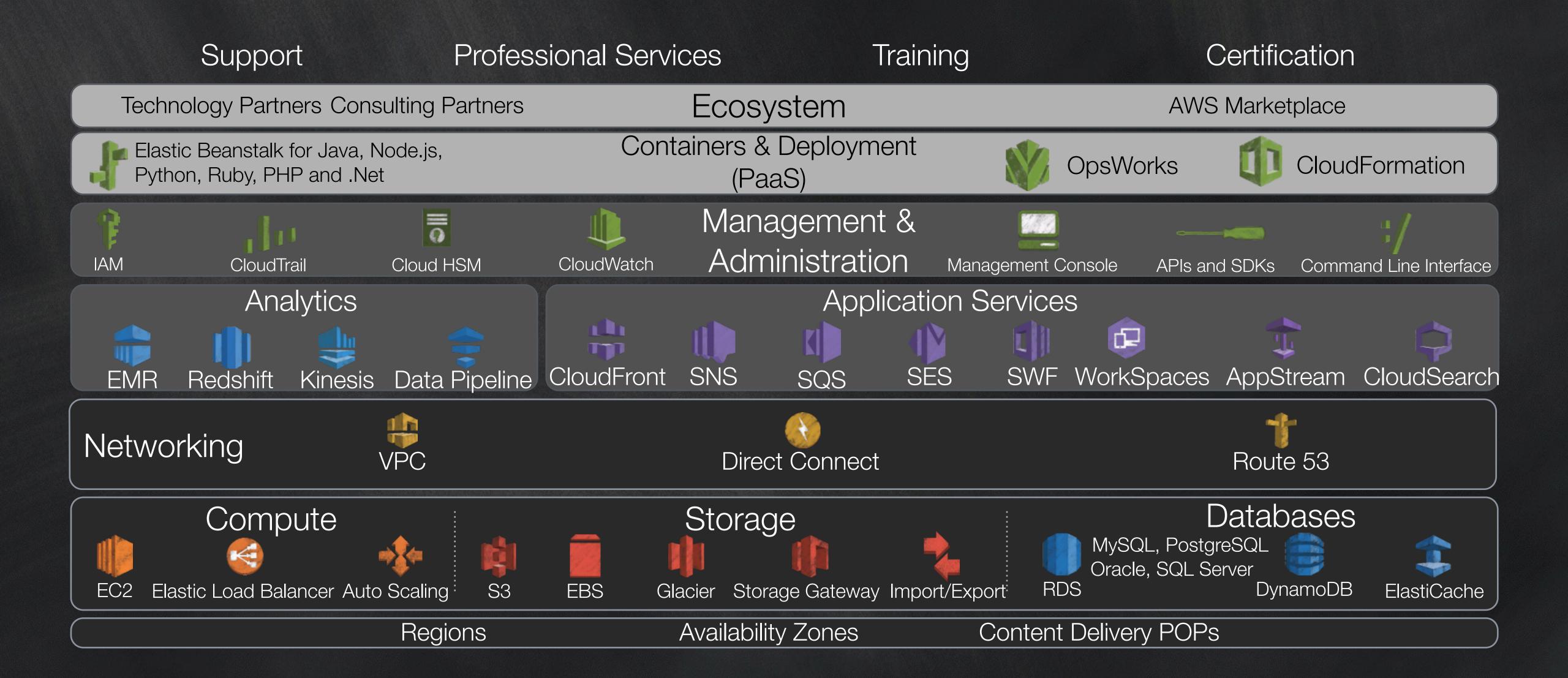












Broad Features and Functionality for Each Service















56 new features since Feb 2013











Regional expansion to US West (Oregon)

Support for temporary credentials when loading data from Amazon S3

Regional expansion to EU West (Dublin)

SOC1/2/3 Compliance certification

Ability to UNLOAD encrypted files in parallel to Amazon S3

Regional expansion to Asia Pacific (Tokyo)

Support for JDBC fetch size to enable extraction of large data sets over JDBC/ODBC

Enable logging of UNLOAD statements

New built-in function to compute the SHA1 hash of a value

Added support for UTF-8 characters up to 4 bytes in size

Ability to share snapshots between accounts to simplify manageability.

Support for statement timeouts to automatically terminate queries that exceeded allotted execution time

Added support for timezone conversion in SQL

Added support for datetime values expressed in milliseconds since EPOCH to simplify ingestion

Simplified ingestion by automatically detecting date and time formats.

Added support for automatic query timeouts to workload management queues.

Enabled the use of wildcards when assigning queries to workload management queues.

New built-in function to enable customers to calculate the CRC32 checksum of a value

Console improvements to show progress bars for backup and restore operations.

Added the ability to support IAM at the resource level allowing tight control of who can take what actions on which resources.

Obtained PCI compliance

Added the ability to substitute a customer chosen character for invalid UTF-8 characters to simplify ingestion

Allowed customers to store JSON data in VARCHAR columns and added built-in functions to enable data extraction

Added support for POSIX regex expressions when using SIMILAR to in SQL queries

Added Cursor support to enable extraction of large data sets over ODBC connections

Built-in function to enable splitting a string using a supplied delimiter to make parsing values easier

Added system tables to enable logging of database activity for auditing

Regional expansion to Asia Pacific (Singapore, Sydney)

Enable customers to control cluster encryption keys by using an on premises hardware security module (HSM) or Amazon CloudHSM Enable customers to receive alerts via SNS for informational or error-related events for cluster monitoring, management, configuration and

Integration with Canal to enable streaming data ingestion

Copy from an arbitrary SSH connection enabling direct copy from Amazon EMR, HDFS, or any other database that supports SSH access and

Enable distributing tables to all compute nodes to speed up queries, especially those involving star or snowflake schemas

Logging of database logins, failed logins, SQL execution and data loads to S3 and integration with CloudTrails for control plane events Enabled caching of database blocks to speed up access to frequently queried data

Increase cluster concurrency limits from 15 to 50 to enable higher concurrent query execution

Optimizations to resize code that lead to 2-4x improvement in resize performance

Approximate COUNT DISTINCT using HyperLogLog giving 10-20x performance improvements with less than 1% error

Enable customers to continuously, automatically and incrementally back up data to a second AWS region for DR

On track to obtain Fedramp certification

Deliver Redshift on SSD instances enabling a lower-cost, high performance entry point

AWS BIS Data Technologies

Amazon RDS



Hosted Relational Databases

Amazon DynamoDB

Amazon Elasticache Amazon Elastic Map Reduce

Amazon Data Pipeline

Amazon Redshift



Managed

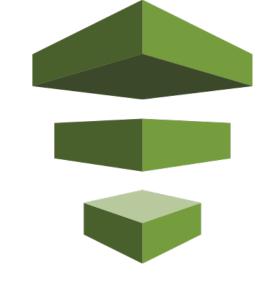
NoSQL

Database



In-memory Caching Service amazon webservices hadoop

Hosted Hadoop framework



Move data among AWS services and onpremise data sources

Petabyte-scale columnar relational data warehouse service

http://aws.amazon.com/big-data/

The AWS Big Data Stack Also Includes...

- o Spark Shark
- o Cassandra
- o Mongobb
- o Pegasus
- o NIT StarCluster

- o Galay
- O GIUSTOI
- o Orangers
- e a a a ma many more

Amazon 53. Over 2 Trillion Total Objects





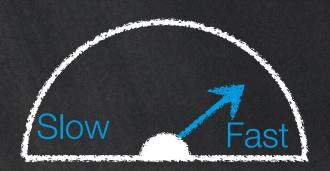
EC2 HPG INSTANCE TYPES

instance type	features	USC CCS		
cg1-GPGPU	2 NVIDIA M2050 2.93GHz Nehalem 22.5gb RAM 2x840gb local storage	GPU based computing CUDA & OpenCL rendering engineering design		
hit - high 10 / SSD	120k random IOPS Intel Xeon 60.5gb RAM 2 x 1tb SSD	databases shared filesystems high IOPS computing		
hs1 - storage	48 TB raw storage Intel Sandy Bridge 117gb RAM 24 x 2tb local storage	large scale data storage node cluster filesystem data warehousing		
cr1 - memory	244gb RAM, AVX, AES-NI 2.6GHz Intel Sandy Bridge with Turbo 2 x 120gb SSD	in memory analytics large cache large memory hoc genome assembly and analytics		

EC2 HPG Instance Types - continued

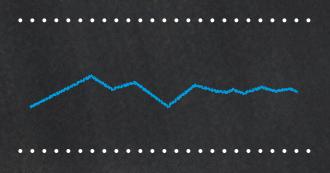
instance type	features	
cc2 - compute	Intel Turbo AVX and AES-NI 2.6GHz Sandy Bridge 60.5 gb RAM 4x840gb local storage	general purpose computing HPC CFD/CAE/MM
g2 - graphics	NVIDIA GK-104 2.6GHz Sandy Bridge 15 gb RAM 60 gb SSD	remote visualization HPC pre-post processing 3d rendering
hi2 - iops / SSD	300,000 random IOPS 2.6 GHz Intel Ivy Bridge - 2/4/8/16/32 VCPU up to 244 gb RAM up to 5.8 tb SSD	large scale data storage node cluster filesystem data warehousing
c3 - compute	turbo to 3.4 Ghz 2.5GHz Ivy Bridge - 2/4/8/16/32 VCPU up to 64 gb RAM up to 640 gb SSD	general purpose computing HPC CAE/CFD/MM
r3 - memory	turbo to 3.4 Ghz 2.5GHz Ivy Bridge - 2/4/8/16/32 VCPU up to 244 gb RAM up to 640 gb SSD	general purpose computing HPC Memory-intensive computing

... Connected by a World-class Network

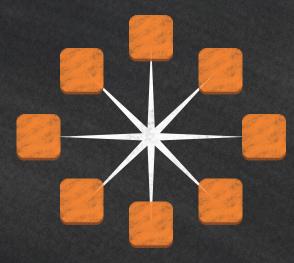


High packets-persecond performance





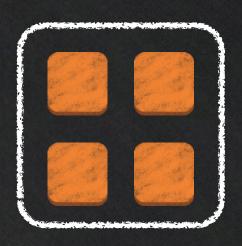
Low jitter



High throughput, low latency



EBS-optimized instances



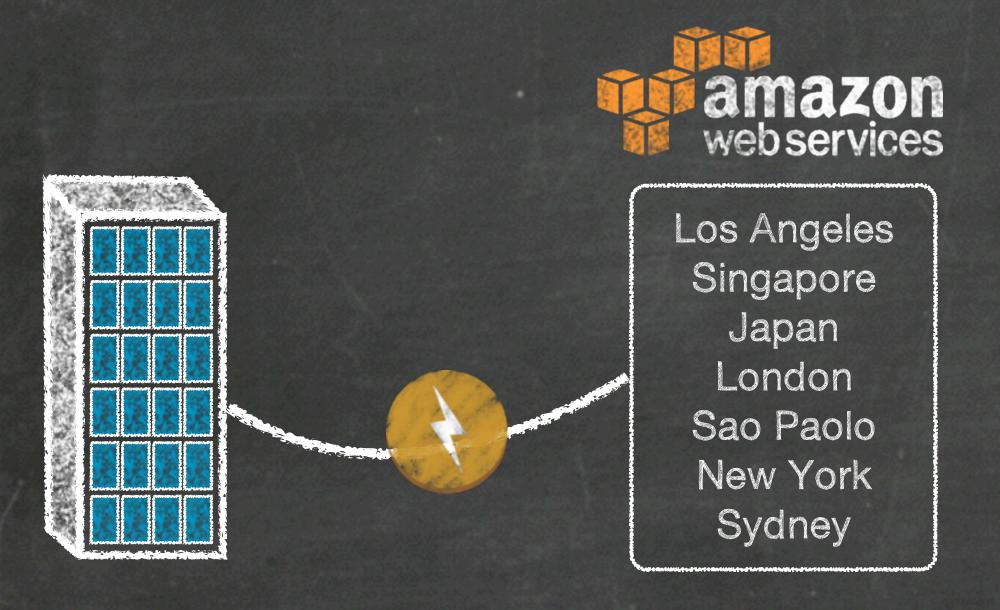
Physical placement optimization

#64 on Top500

	Academy of Sciences China	GHz, Infiniband QDR, NVIDIA 2050 IPE, Nvidia, Tyan				
64	Amazon Web Services United States	Amazon EC2 C3 Instance cluster - Amazon EC2 Cluster, Intel Xeon E5-2680v2 10C 2.800GHz, 10G Ethernet Self-made	26496	484.2	593.5	
65	United Kingdom Meteorological Office United Kingdom	Power 775, POWER7 8C 3.836GHz, Custom Interconnect	18432	476.3	565.6	1040

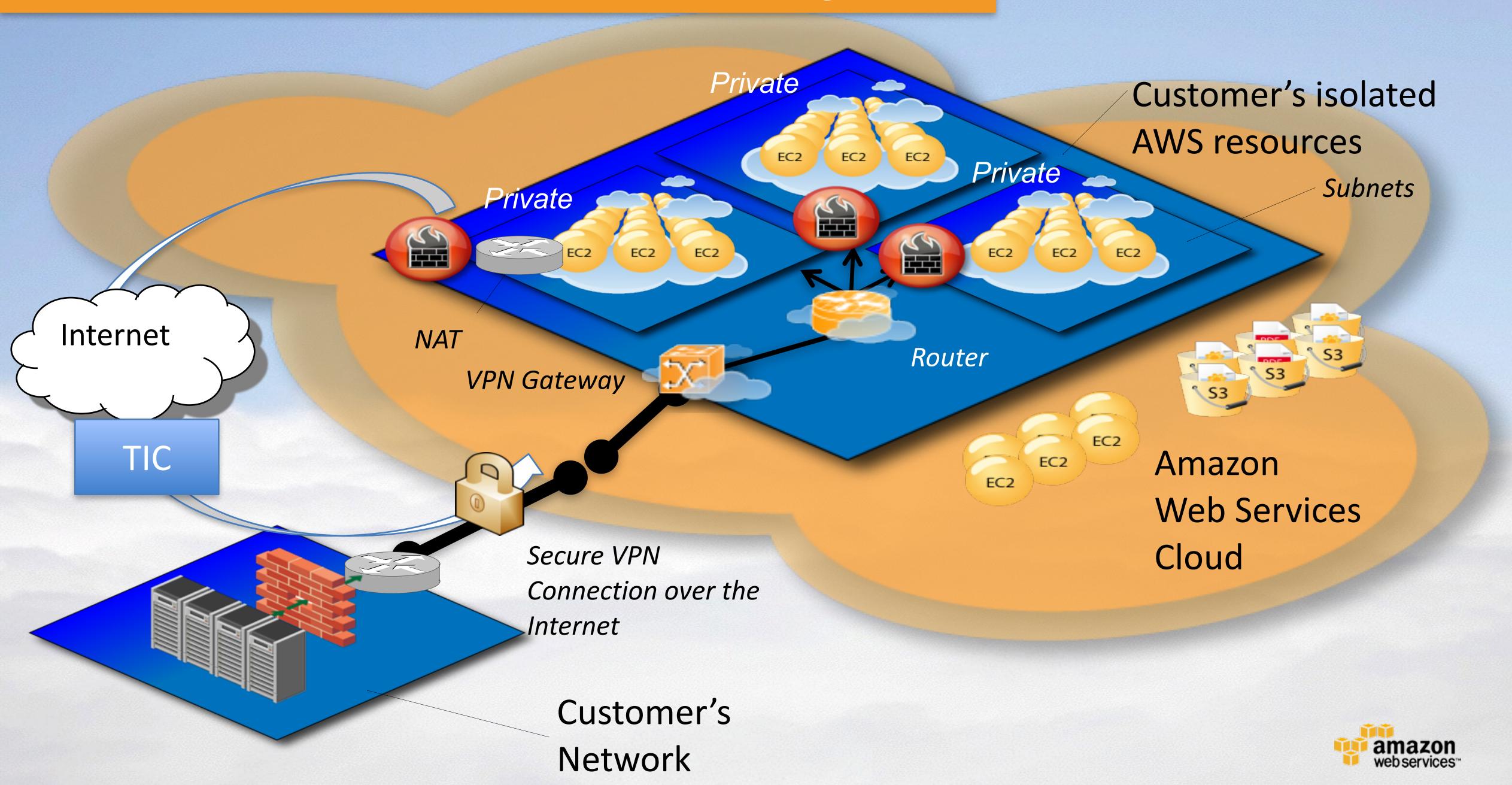
http://top500.org/1st/2013/11/

Integrated Architectures



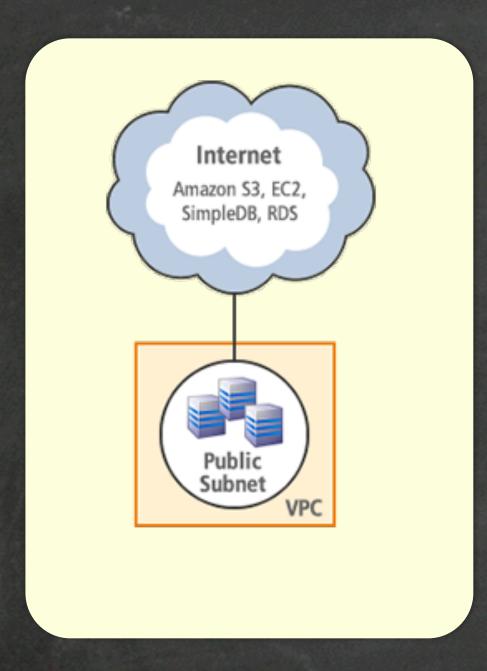


AWS Virtual Private Cloud Networking



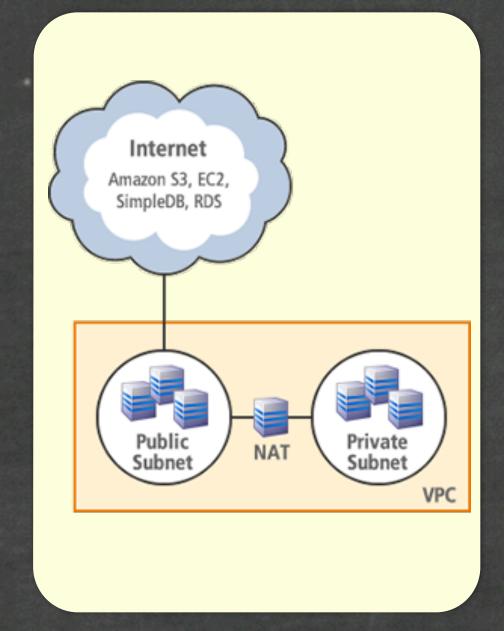
VPC Deployment Models

WPC With a Single Subnet



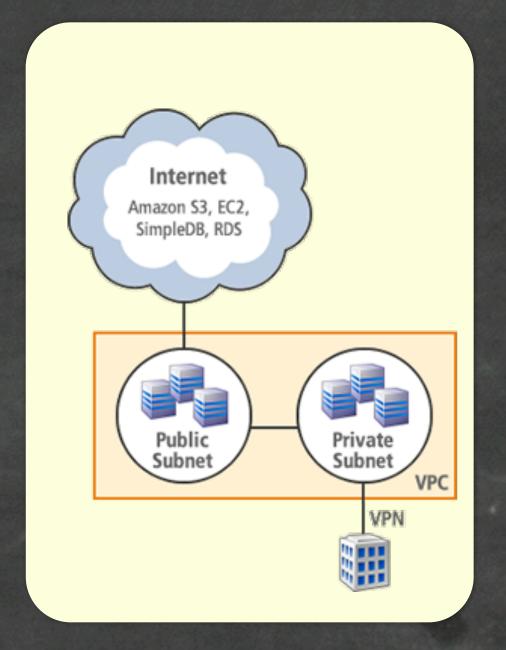
Simple web hosting, collaborative research environments, ondemand HPC/HTC clusters

VPC With Private and Public Subnets



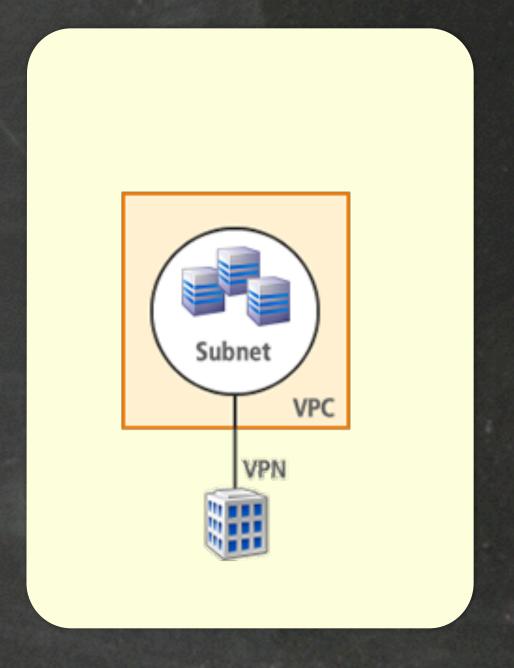
Multi-tier web hosting

VPC With Private and Public Subnets & Hardware VPN access



Multi-tier web hosting with access to internal infrastructure

VPC With a
Private Subnet Only &
Hardware VPN Access



Seamless private expansion of on-premise infrastructure. "Burst capacity" or dedicated cloud environments with connectivity to on-premise resources

Multiple Purchase Models

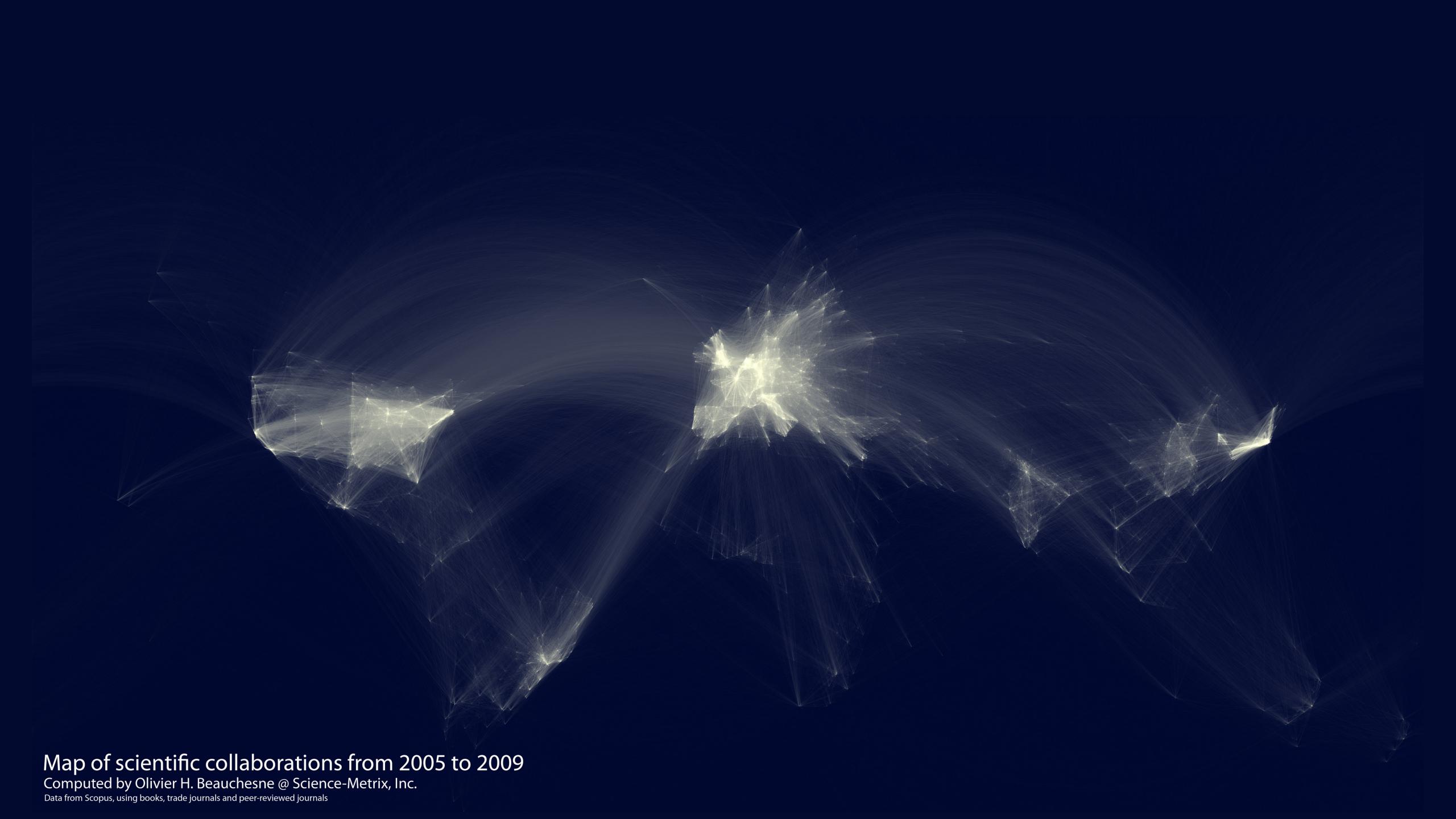
get started on AWS with free usage & no commitment	pay for compute capacity by the hour with no long-term commitments	make a low, one-time payment and receive a significant discount on the hourly charge	bid for unused capacity, charged at a Spot Price which fluctuates based on supply and demand	launch instances within Amazon VPC that run on hardware dedicated to a single customer
for POCs and getting started	for spiky workloads, or to define needs	for committed utilization	for time-insensitive or transient workloads	for highly-sensitive or compliance-relayed workloads

Scientific Computing Use Cases

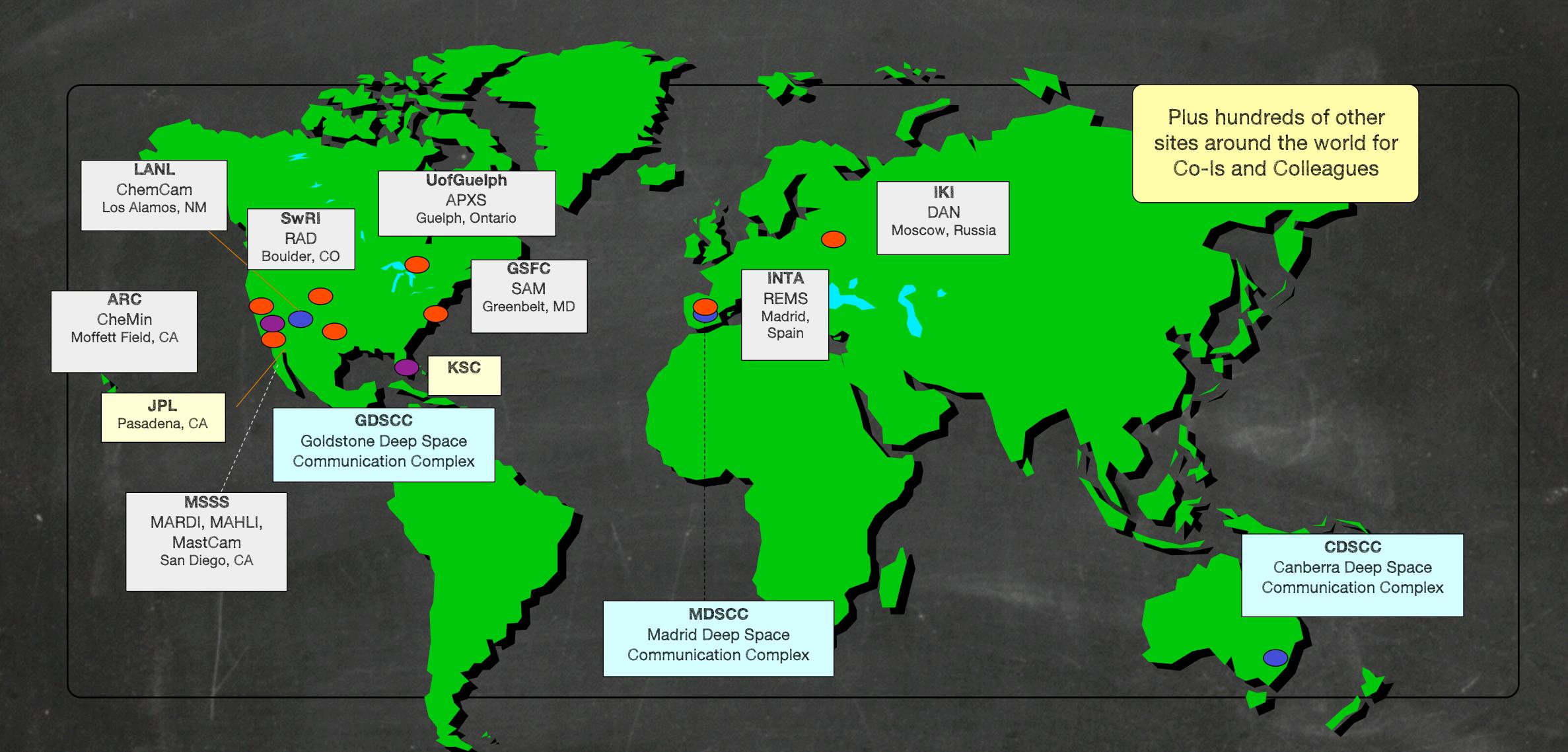
- o Science-as-a-Service
- o Large-scale HTC (100,000+ core clusters)
- Large-scale MapReduce (Hadoop/Spark/Shark) using EC2 or EMR
- Small to medium-scale clusters (hundreds of nodes) for traditional MPI workloads
- Many small MPI clusters working in parallel to explore parameter space
- o Small to medium scale GPGPU workloads
- Dev/test of MPI workloads prior to submitting to supercomputing centers
- Ephemeral clusters, custom tailored to the task at hand, created for various stages of a pipeline
- o Collaborative research environments
- o On-demand academic training/lab environments

Who is using AWS?



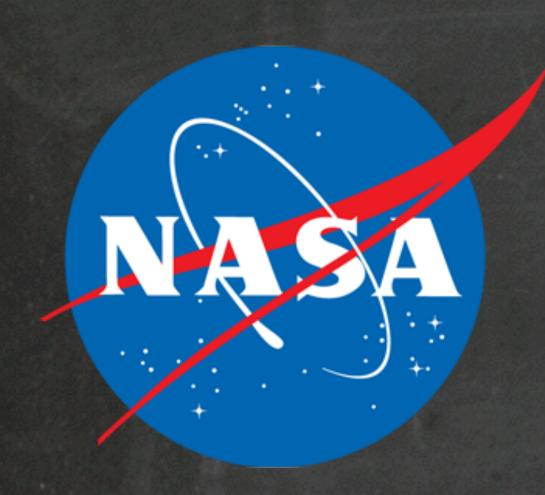


MSL Distributed Operations



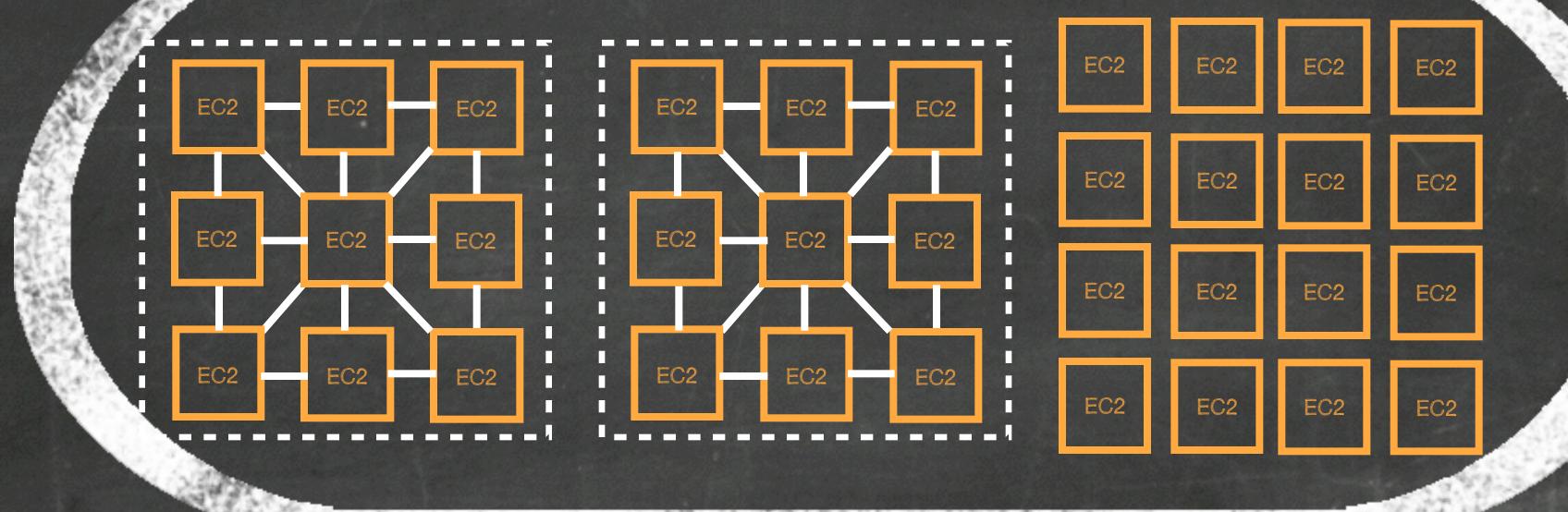




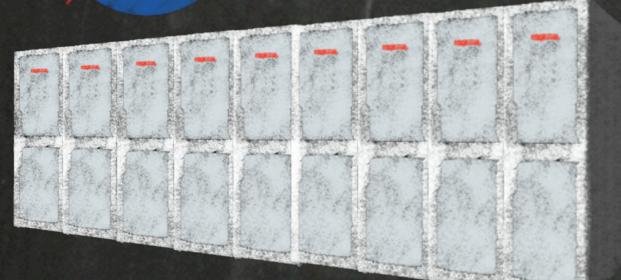


Jet Propulsion Laboratory California Institute of Technology









On-demand access to effectively limitless resources

Specialized supercomputing resources

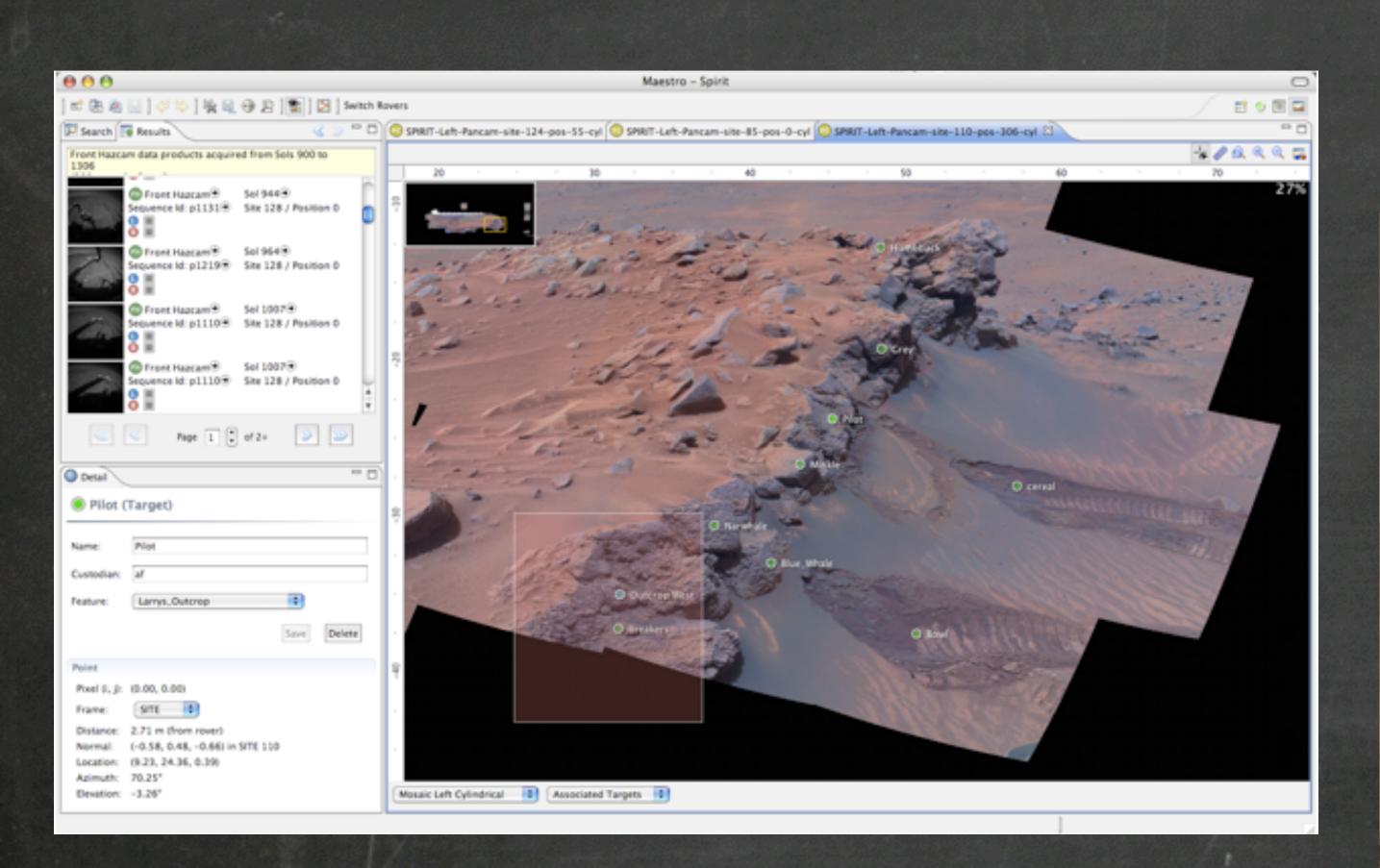


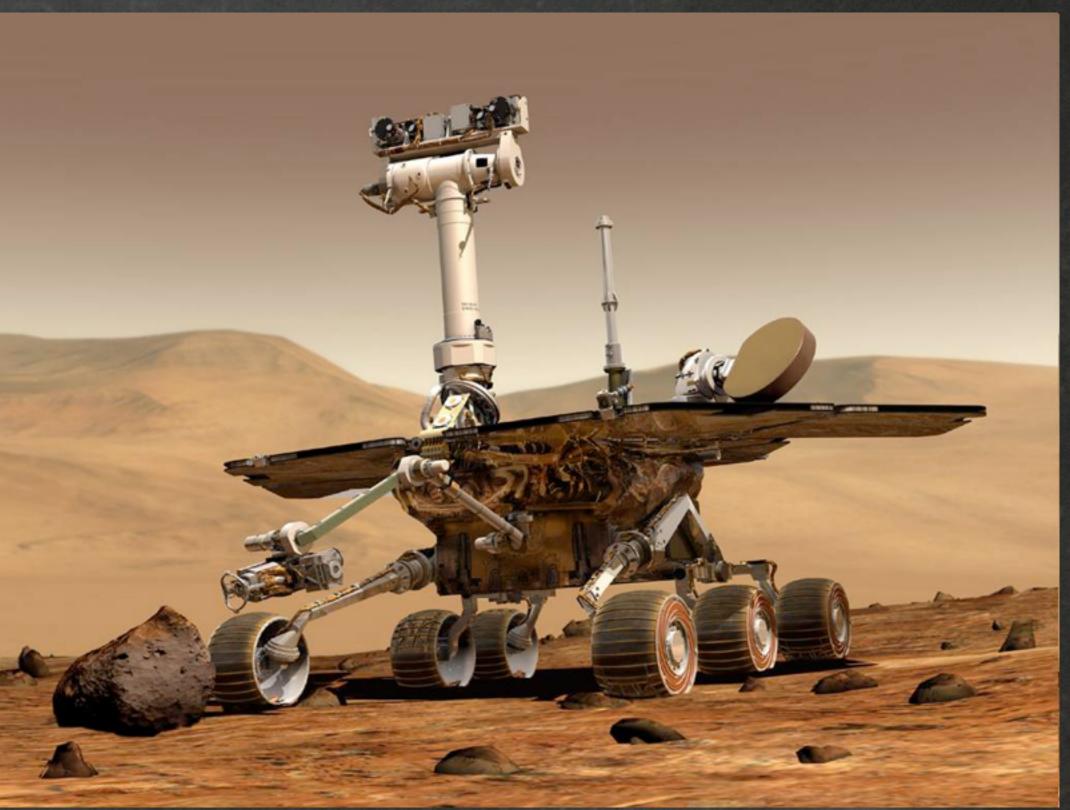


Small-scale shared compute



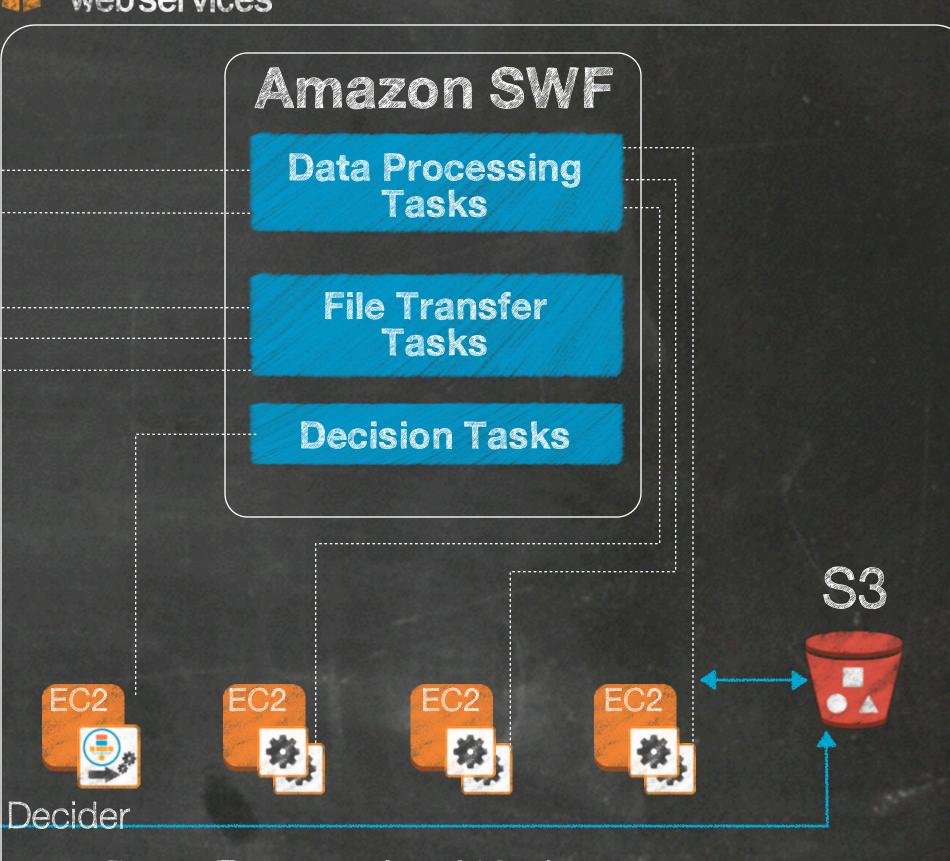
Mission-Critical Computing







JPL Data Center amazon Amazon SWF Data Processing Data Processing Tasks Workers Transfer a second distance of the second second distance of the second second second second second second second second File Transfer Tasks Workers **Decision Tasks** Decider Create EC2 袋 Instances Decider Data Processing Workers Upload and Polyphony Download File Chunks



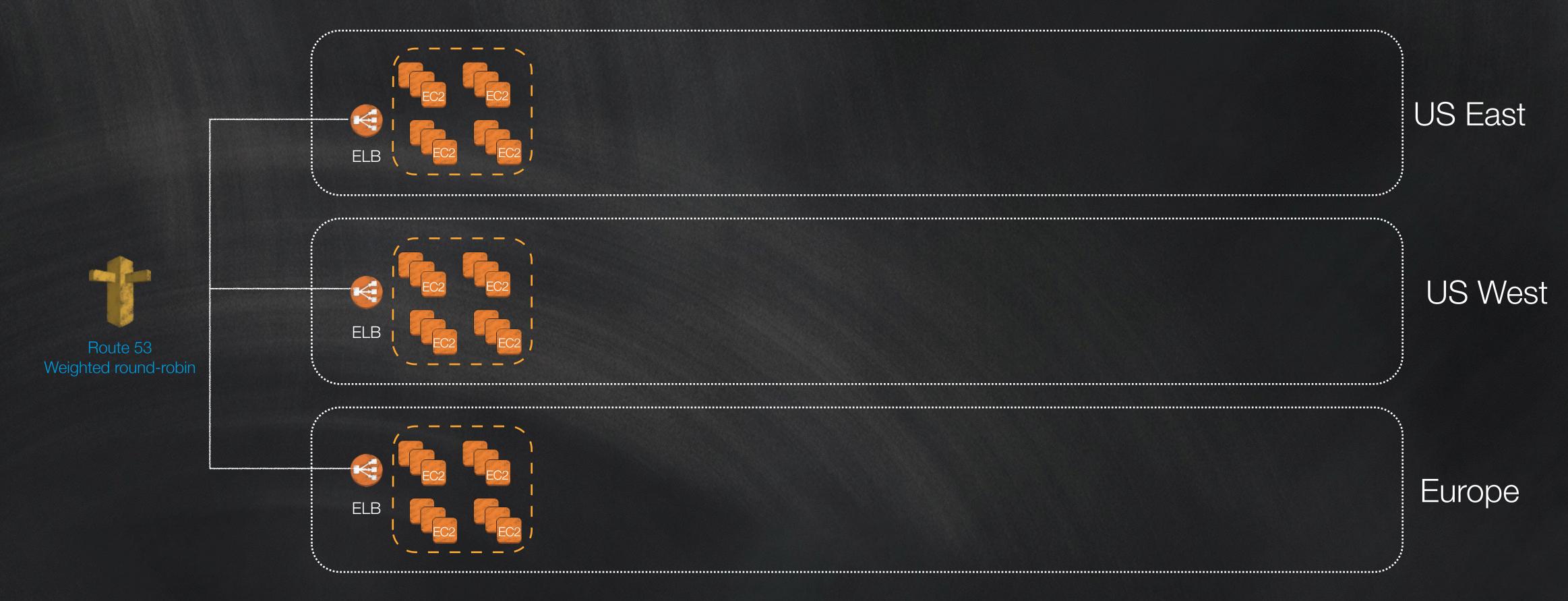




Route 53: Multi-region weighted round-robin distribution

AWS Marketplace: Pre-configured Adobe Flash Media Server

Curiosity live stream



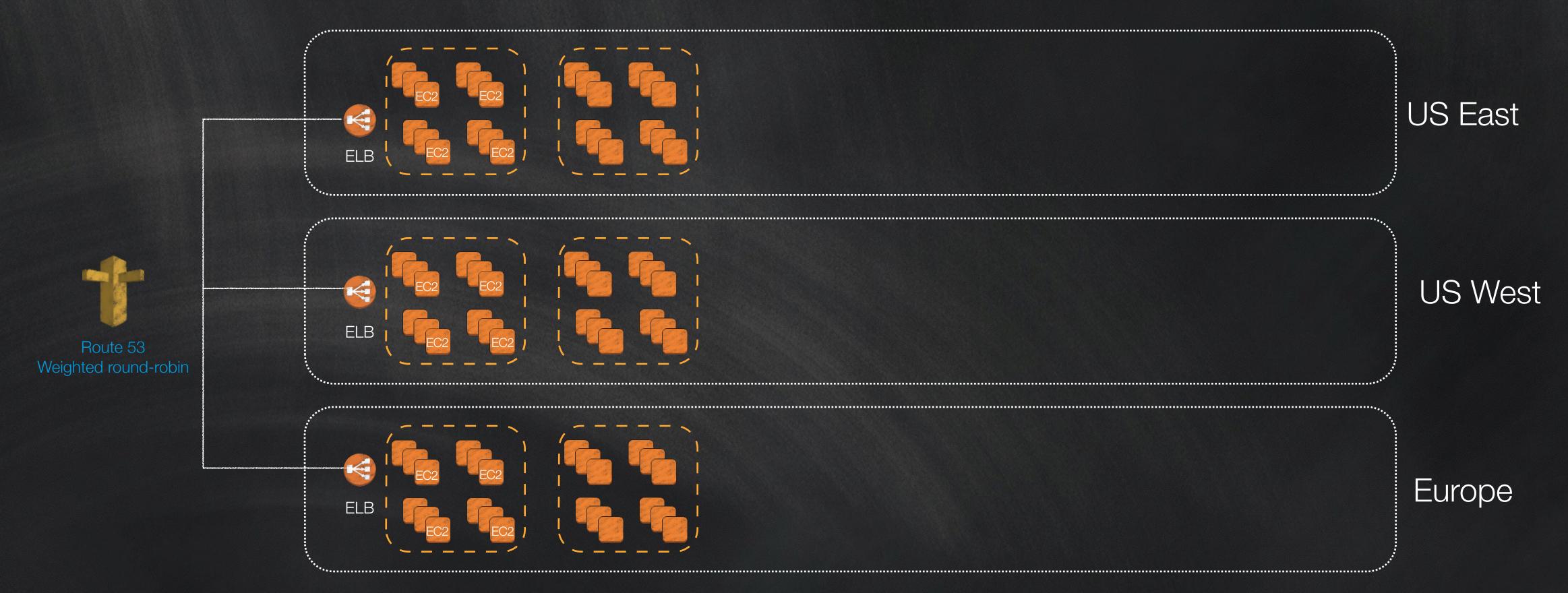


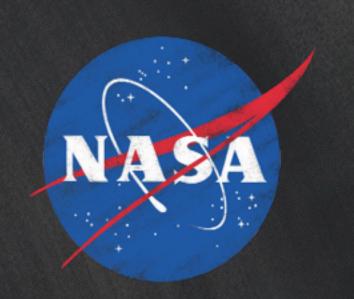
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CloudFormation: Quickly deploy repeatable units of streaming capacity

Curiosity live stream





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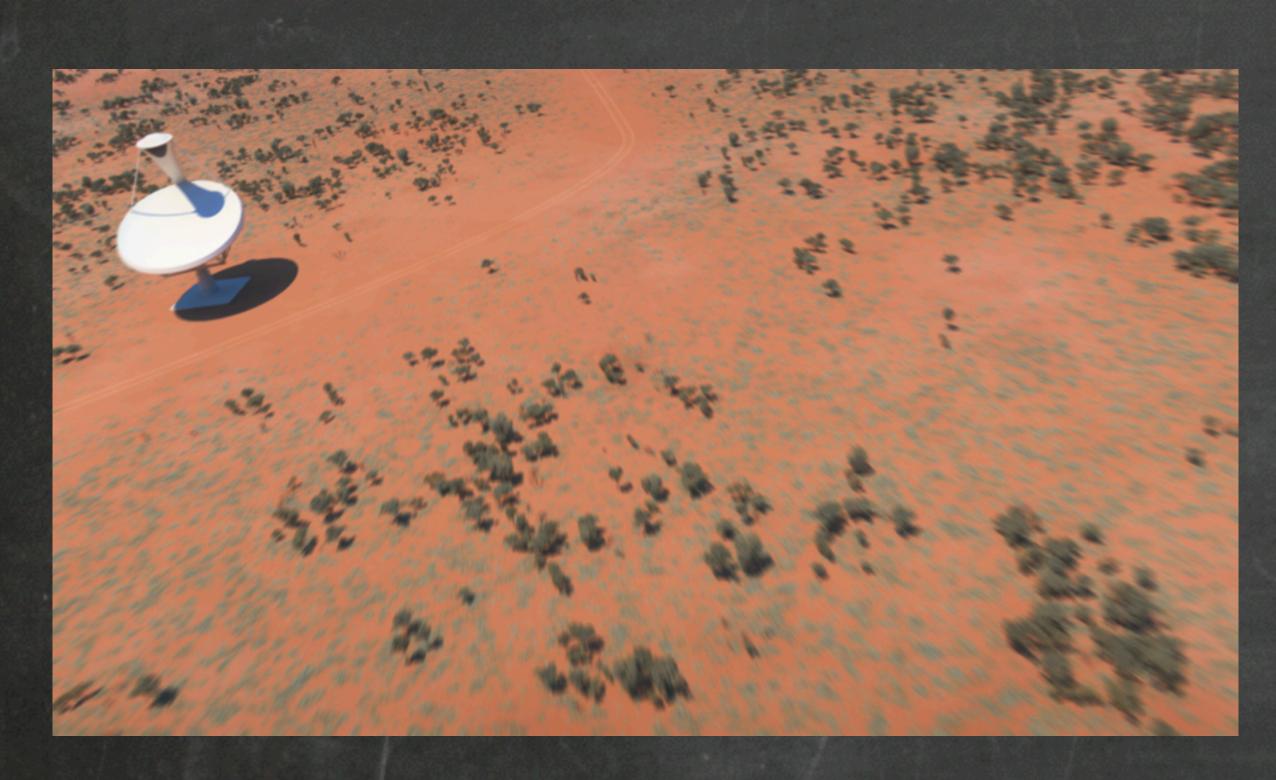
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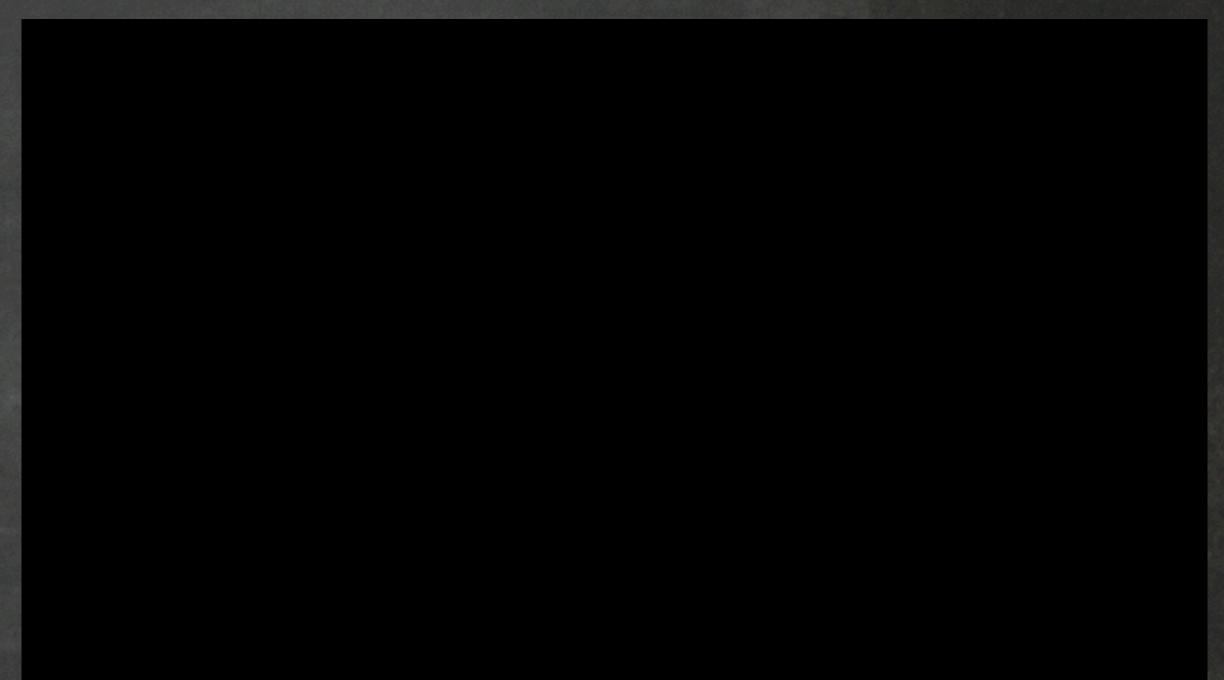
Curiosity live stream



The Square Kilometer Array







SMAJON DIPOLES

SCALING MINA/ASKAP TO SKAL

	MWA	ASKAP	SKA1-SURVEY	SKA1-LOW	SKA1-MID
Digitiser Output	0.12 Tbit/s	69 Tbit/s	184 Tbit/s	10 Tbit/s [3]	17.1 Tbit/s [1]
	1x	575x	1533x	83x	143x
Input to	3.2 Gbit/s	20 Gbit/s	37360 Gbit/s [2]	6736 Gbit/s [2]	26000 Gbit/s [2]
Science Data Processor	1x	6.3x	11675x	2105x	8125x
Archived Science Data Products	3 PB/year (25% duty cycle) [4]	5 PB/year	Exabytes per year	Exabytes per year	Exabytes per year

^[1] From SADT Consortium Technical Development Plan (SKA-TEL.SADT-PROP_TECH-RED-001)

^[2] From SKA1 System Baseline Design (SKA-TEL-SKO-DD-001)

^[3] From LFAA Technical Description (AADC-TEL.LFAA.SE.MGT-AADC-PL-002)

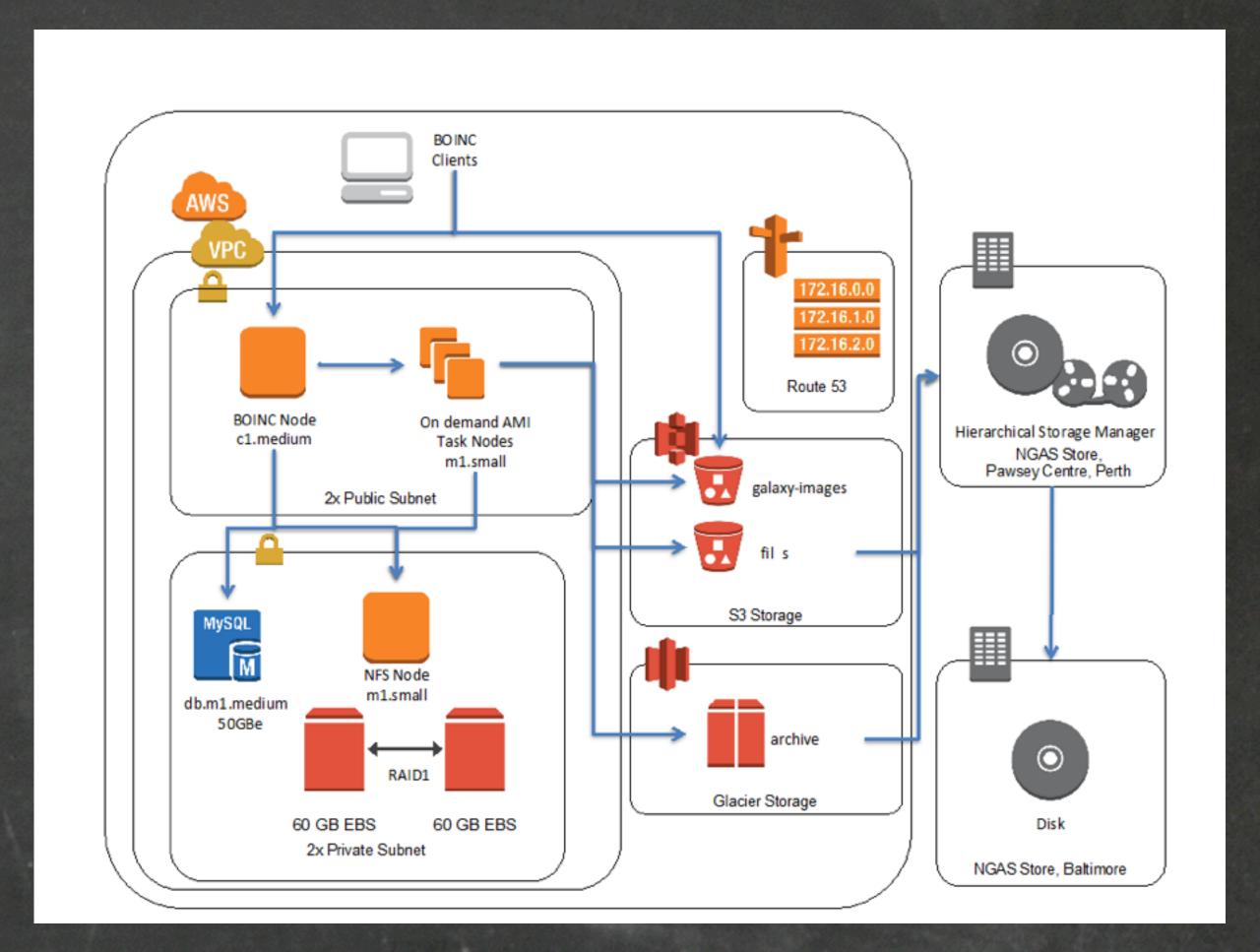
^[4] MWA is archiving correlator output data, not science data processor output data



Skyllet - ICRAR EPO System for the SKA

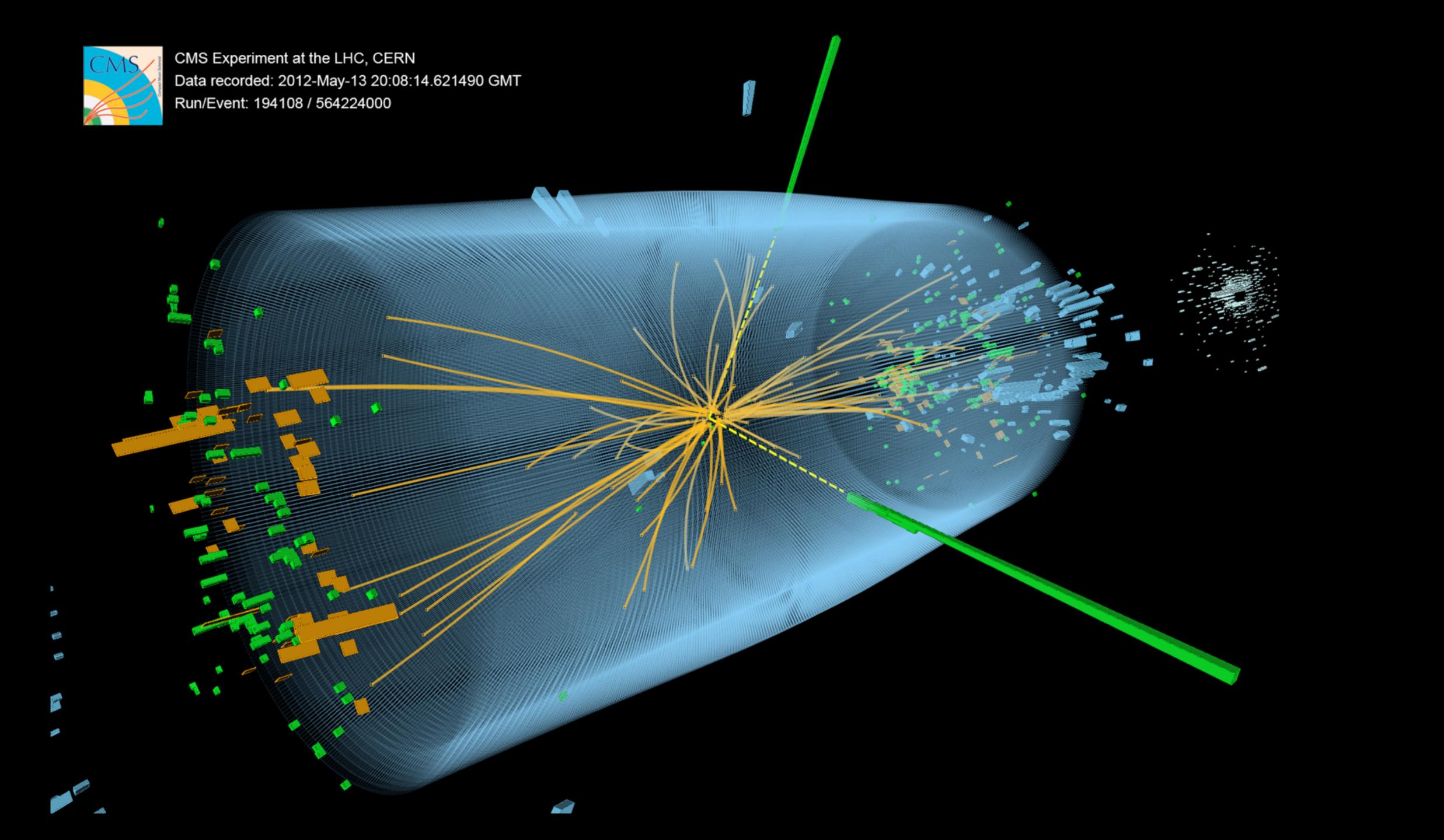


International Centre for Radio Astronomy Research



ICRAR SkyNet Architecture

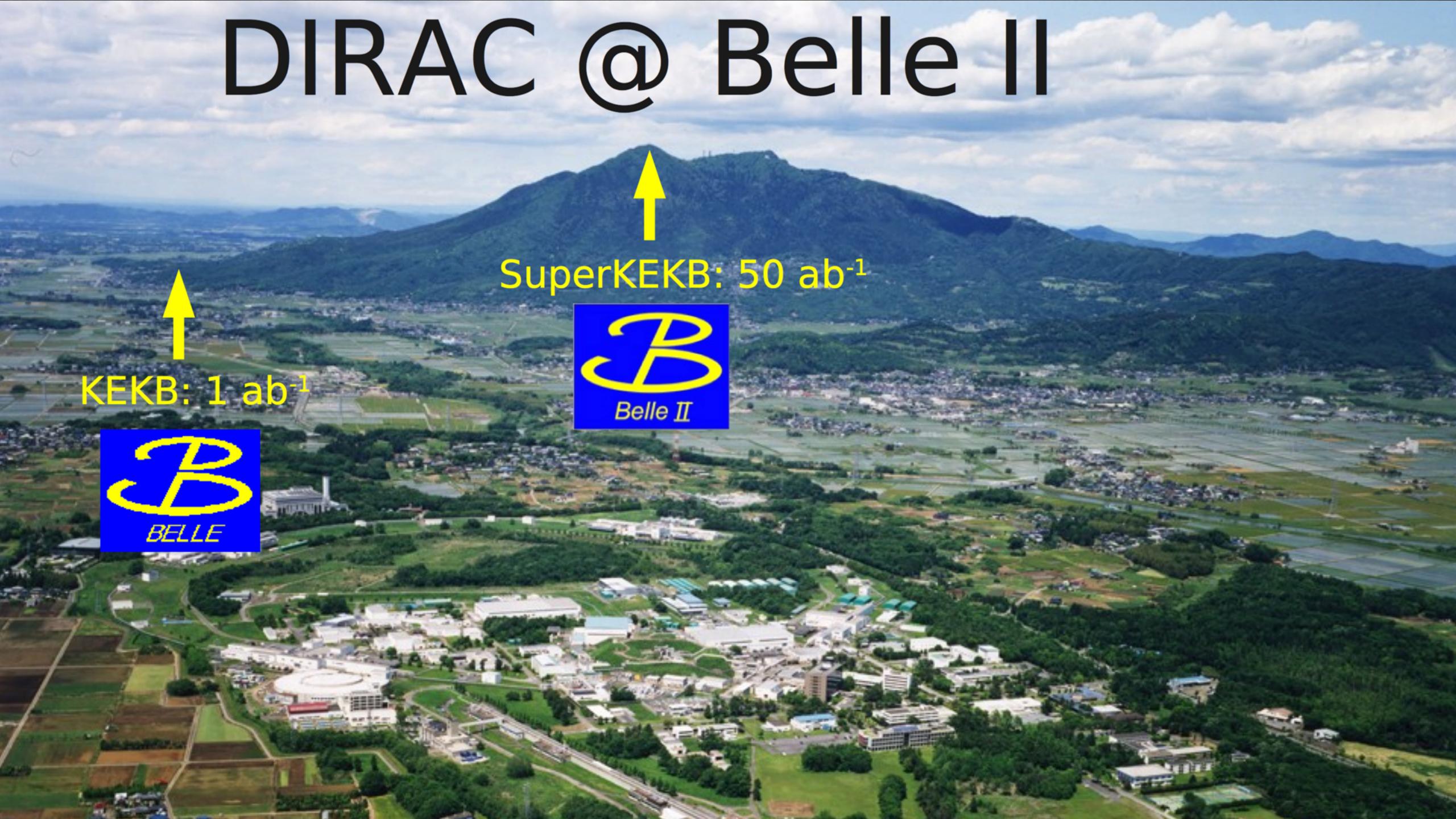
http://aws.amazon.com/solutions/case-studies/icrar/

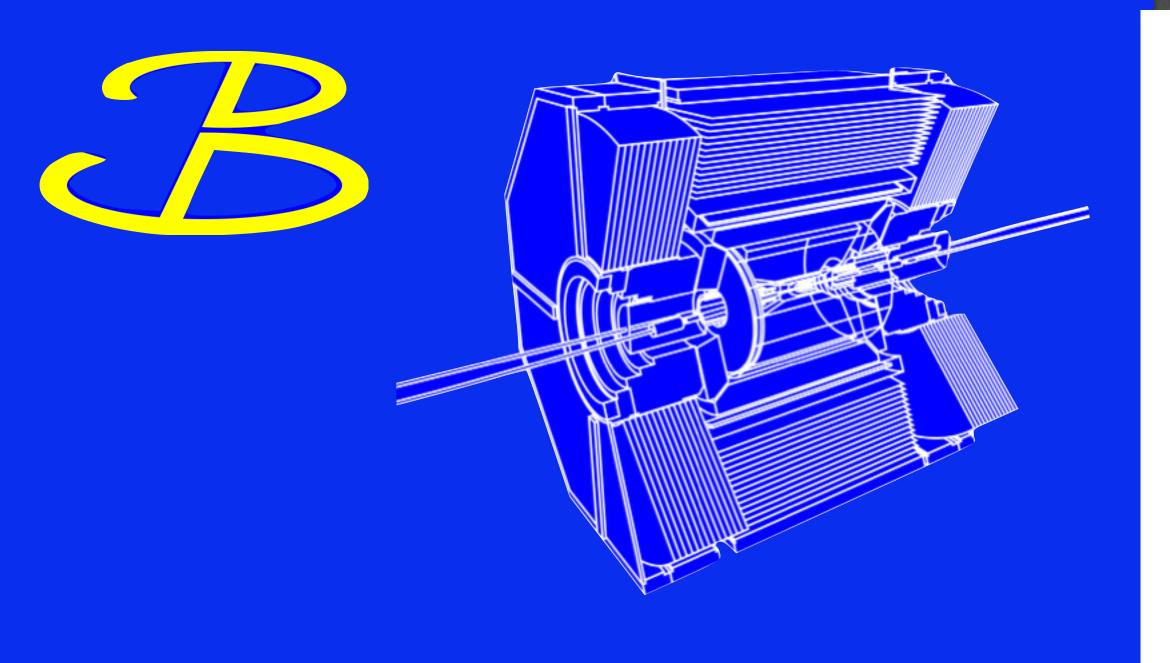


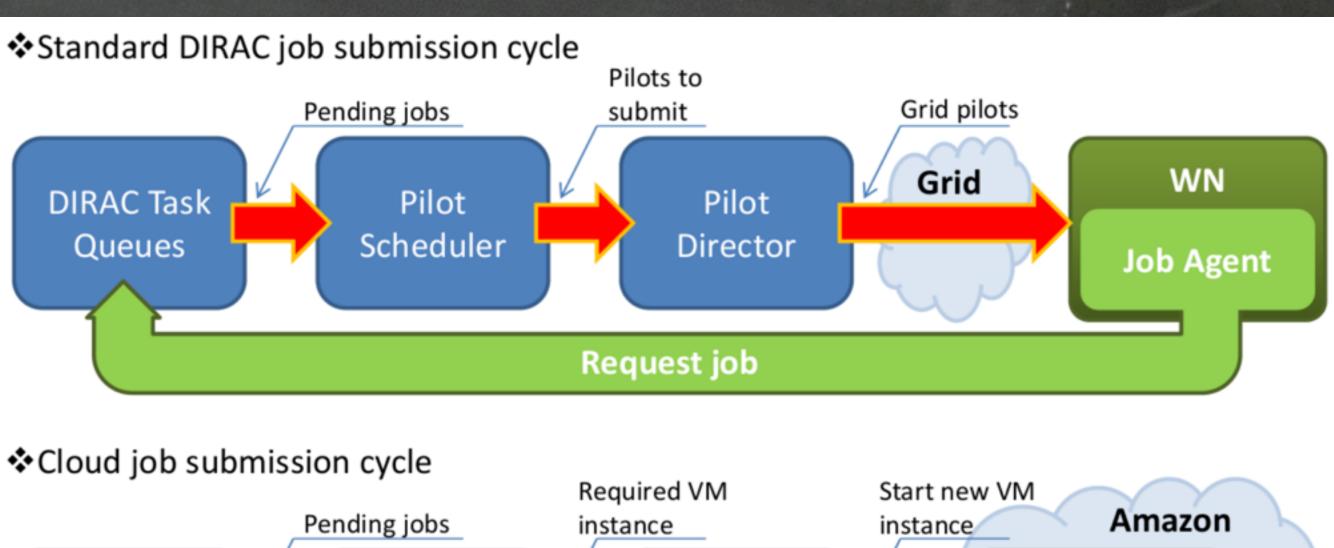
Globaly Distributed Compute for LHC on Amazon EC2 Spot



http://www.hep.wisc.edu/~dan/talks/EC2SpotForCMS.pdf







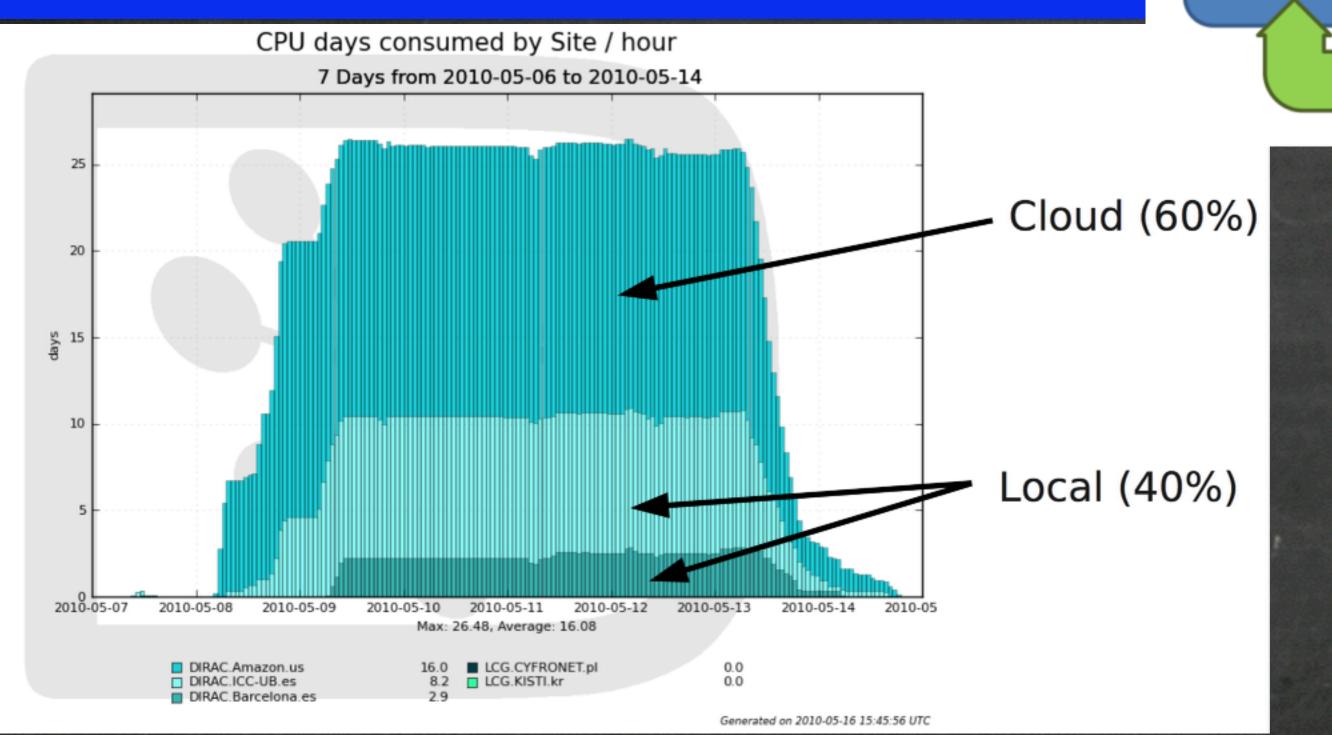
Virtual

Machine

Scheduler

DIRAC Task

Queues



Hybrid Computation Model

Request job

Amazon

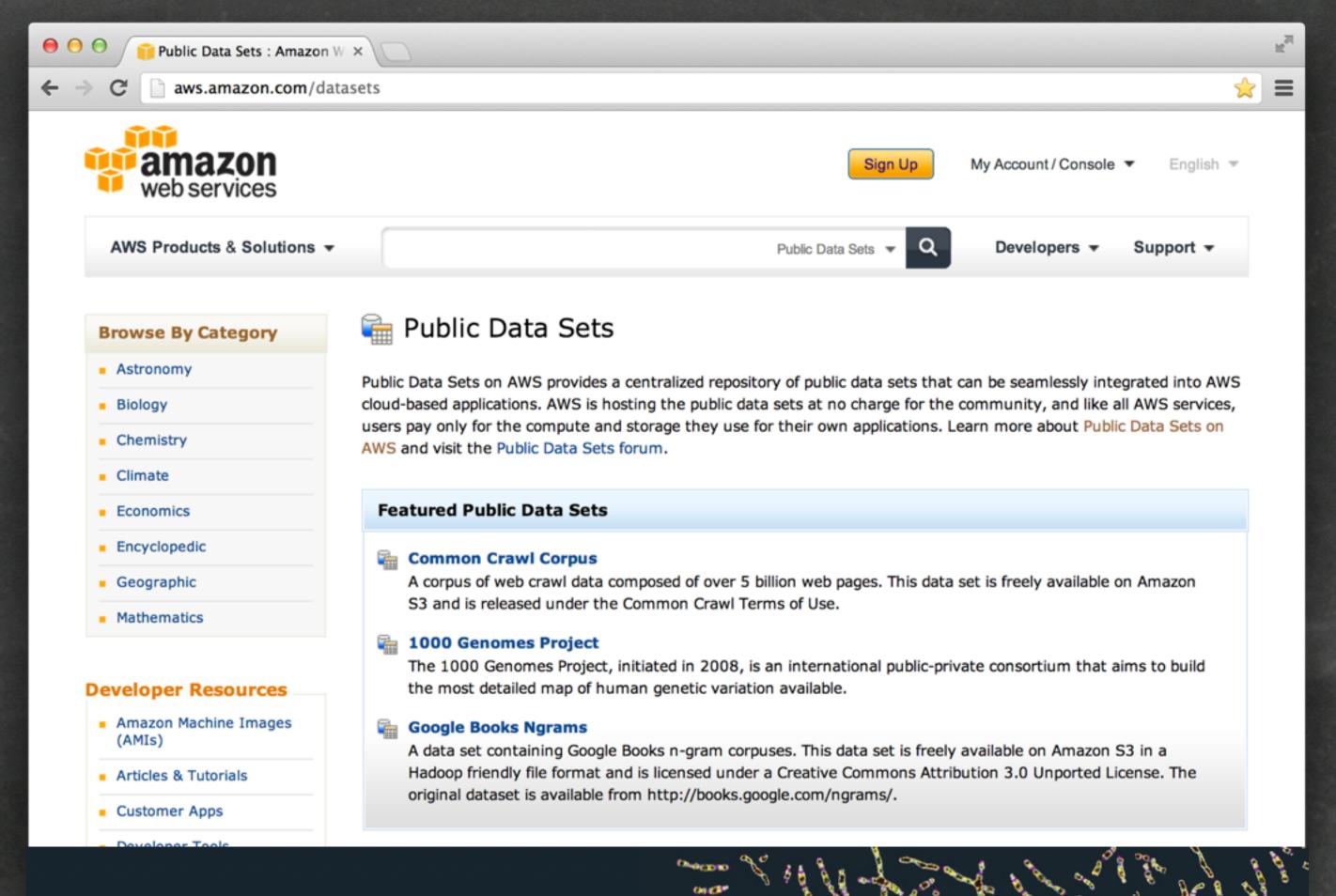
Director

WN

Job Agent

- <- Belle on AWS Price/Performance Benchmark
- 170M events (3.6 TB) produced in 6 days
- Amazon Spot Instances -> \$0.20 / 10k events
 (May, 2010 pricing)

AWS PUDIC Data Sets



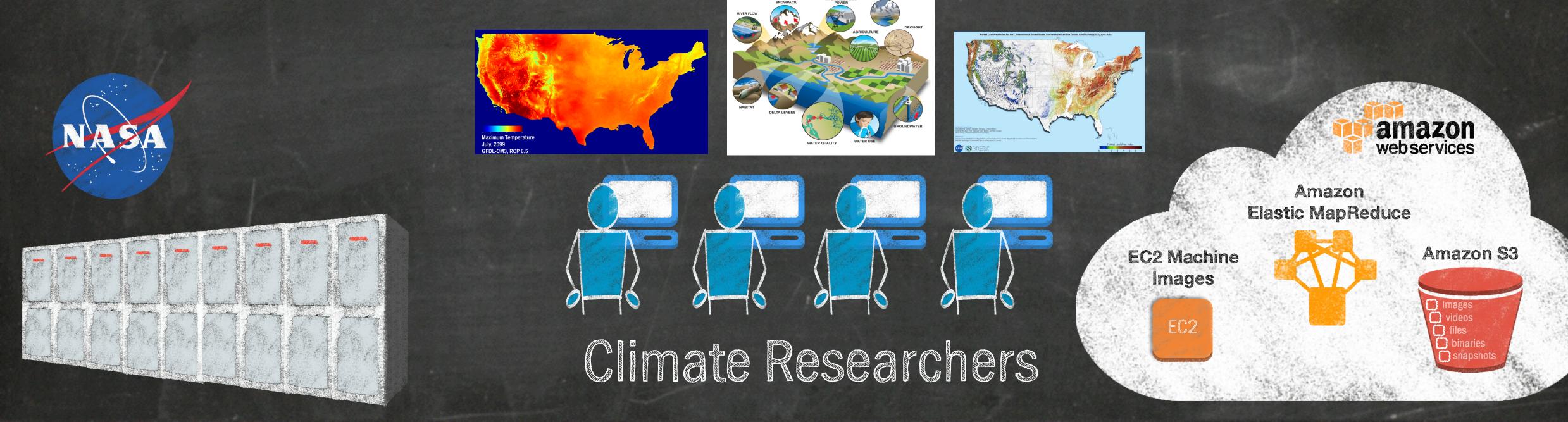
1000 Genomes

A Deep Catalog of Human Genetic Variation

AWS.amazon.com/datasets

AWS and the NASA Earth exchange (NEX)

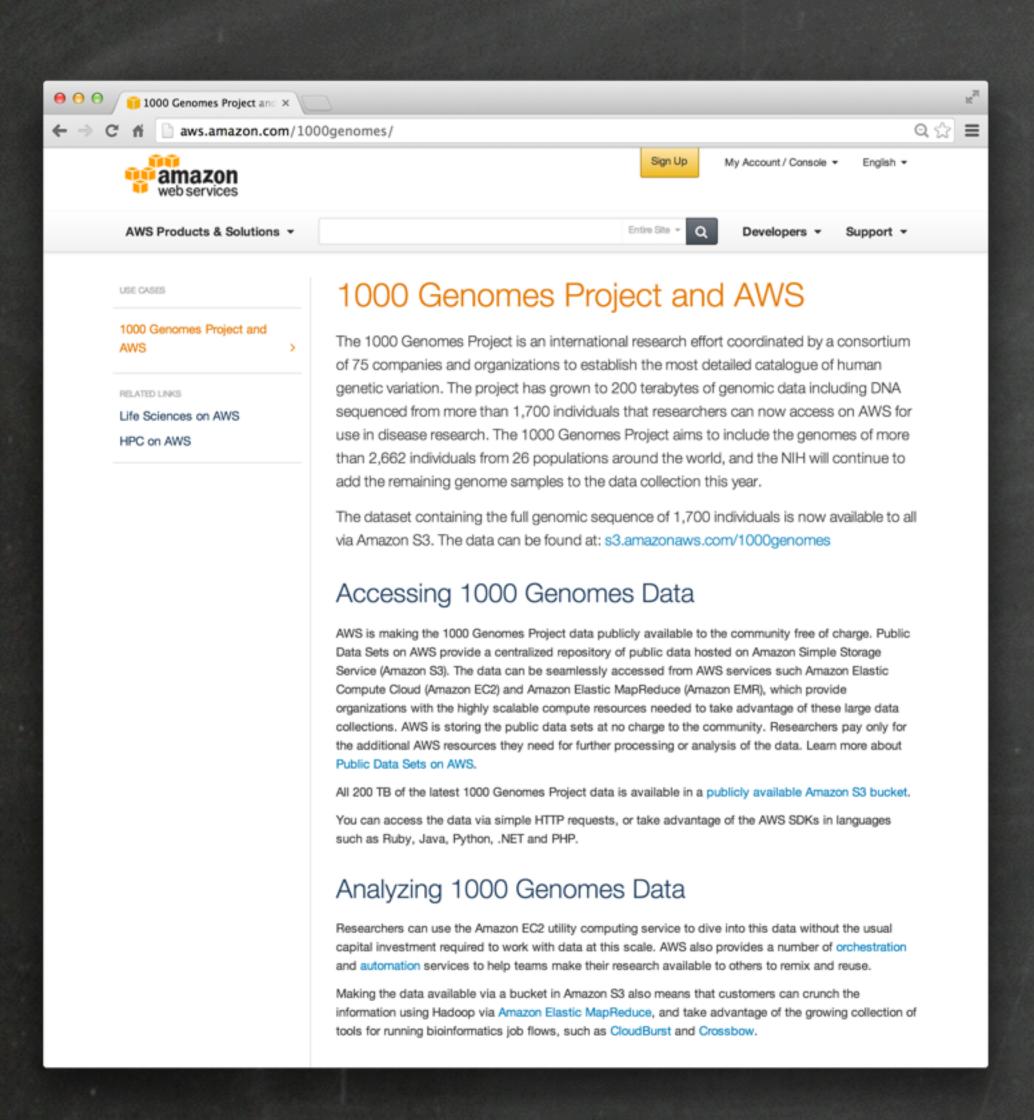
- National Climate Assesment datasets hosted on AWS
- Machine images, tutorials and hosted workshops provided by NASA
- o Data and Software now available to those without @nasa.gov email addresses
- Enables crowd-sourced citizen science applications like those found on the Zooniverse

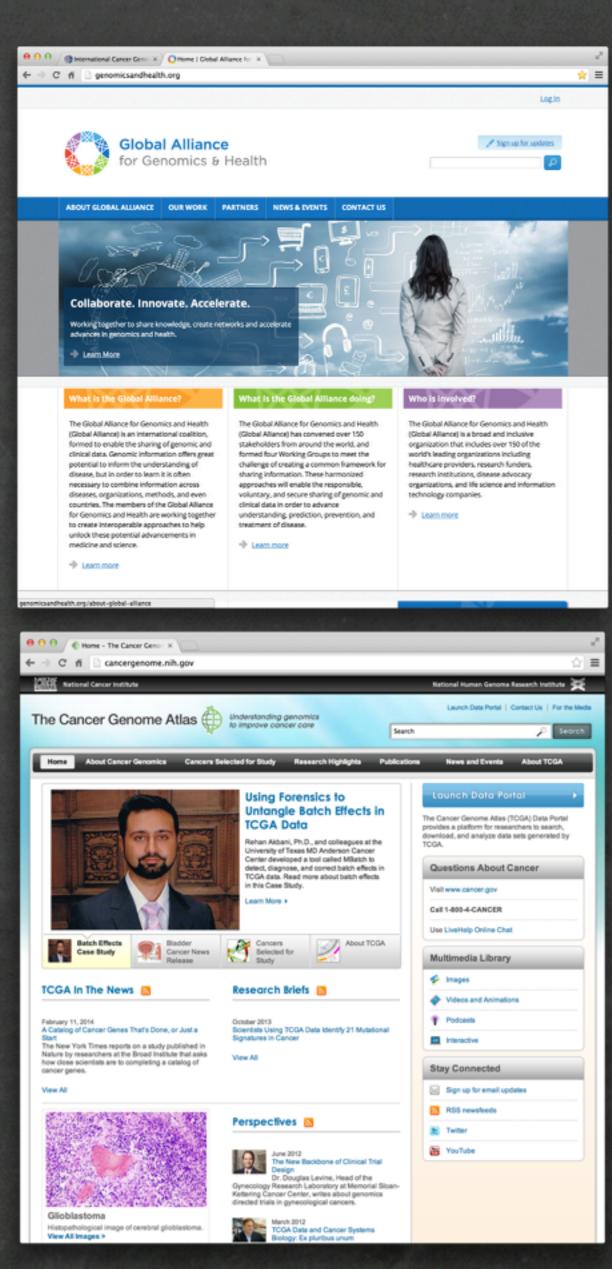


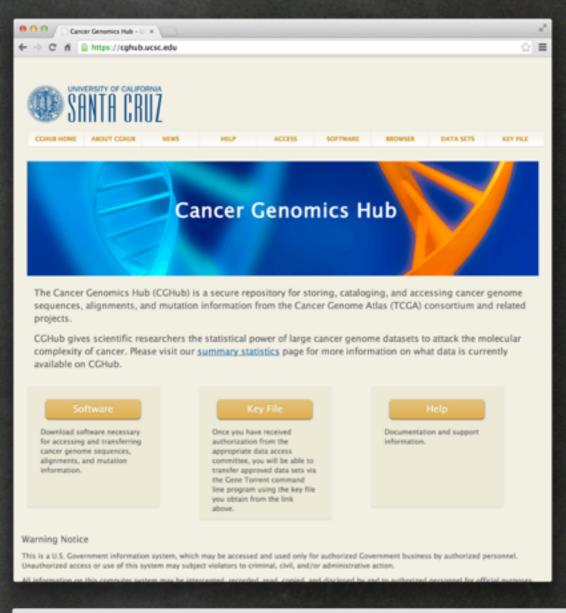
Multi-Spectrum Atlas of the Galactic Plane

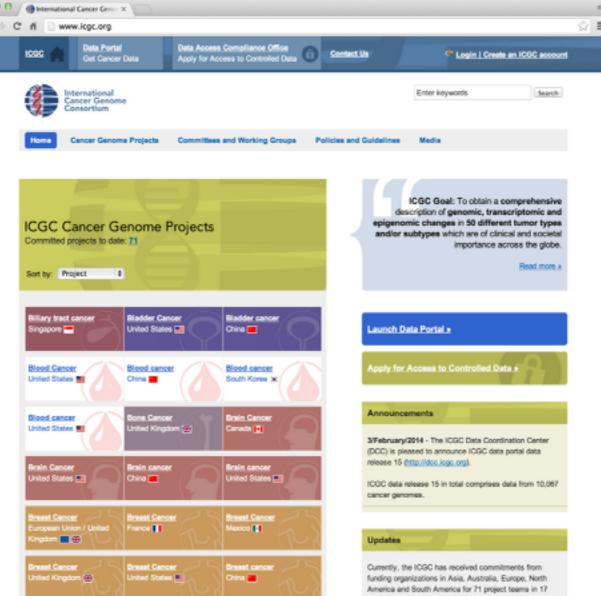
- Collaboration between AMS, Caltech/IPAC and USC/ISI
- All images are publicly accessible via direct download and VAO APIS
- o 16 wavelength infrared atlas spanning 1 µm to 70 µm
- o Datasets from GLIMPSE and MIPSGAL, 2MASS, MSX, WISE
- Spatial sampling of 1 arcsec with ± 180° longitude and ± 20° latitude
- o Mosaics generated by Caltech's Montage (http://montage.ipac.caltech.edu)
- Compute resources coordinated by USC's Pegasus (http://pegasus.isi.edu/)

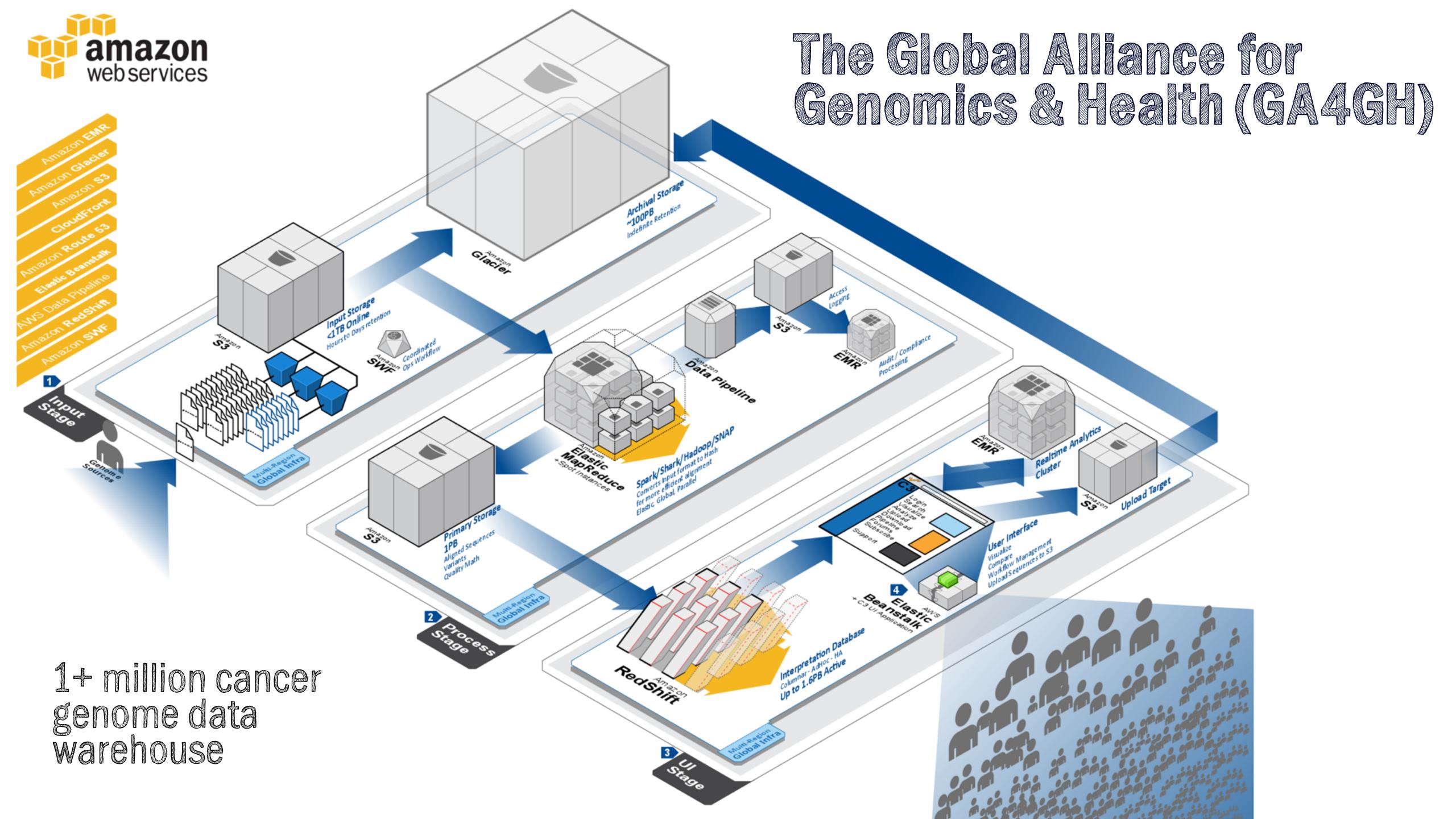
Cancer Research with AWS











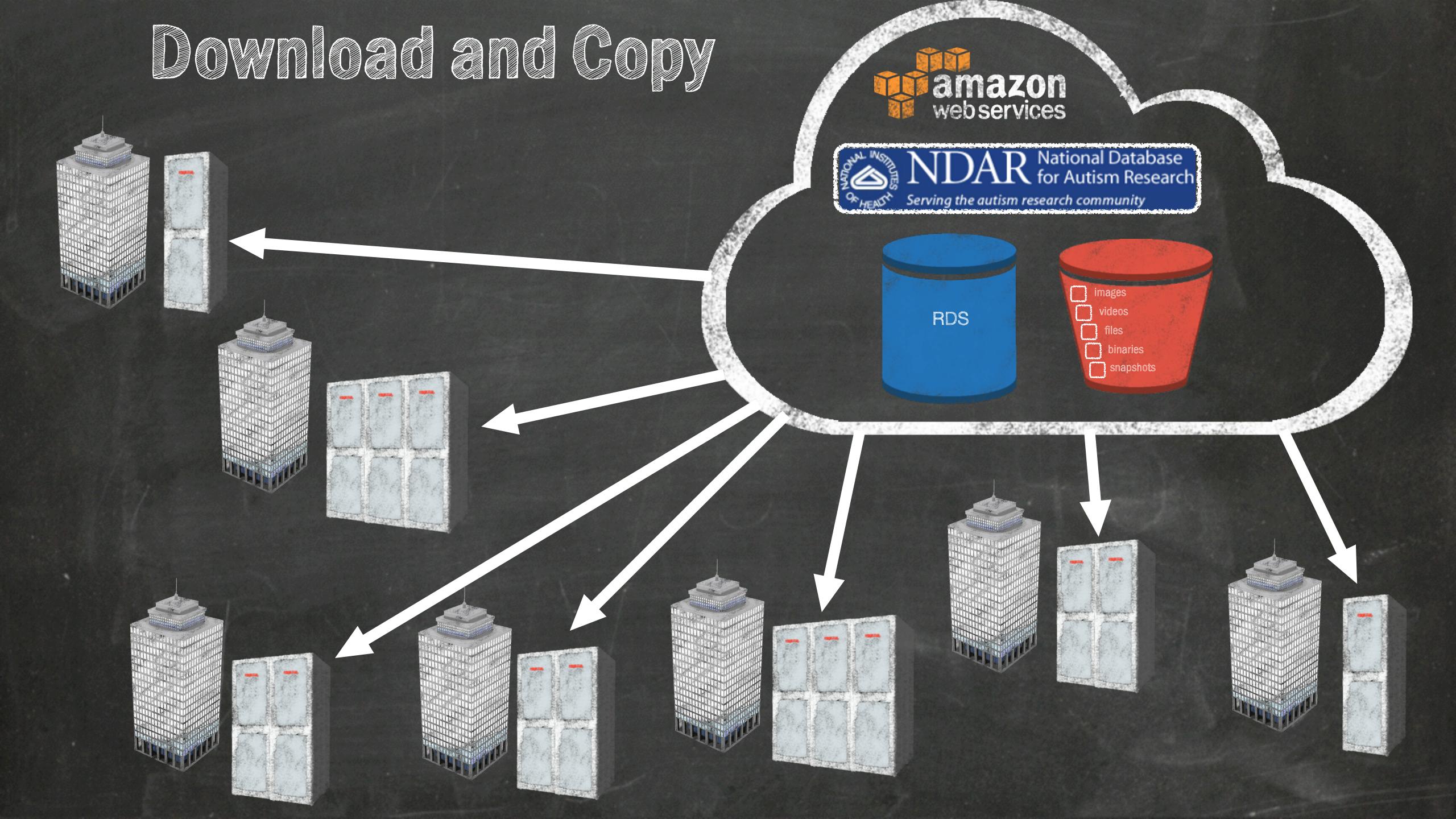
National Database for Autism Research

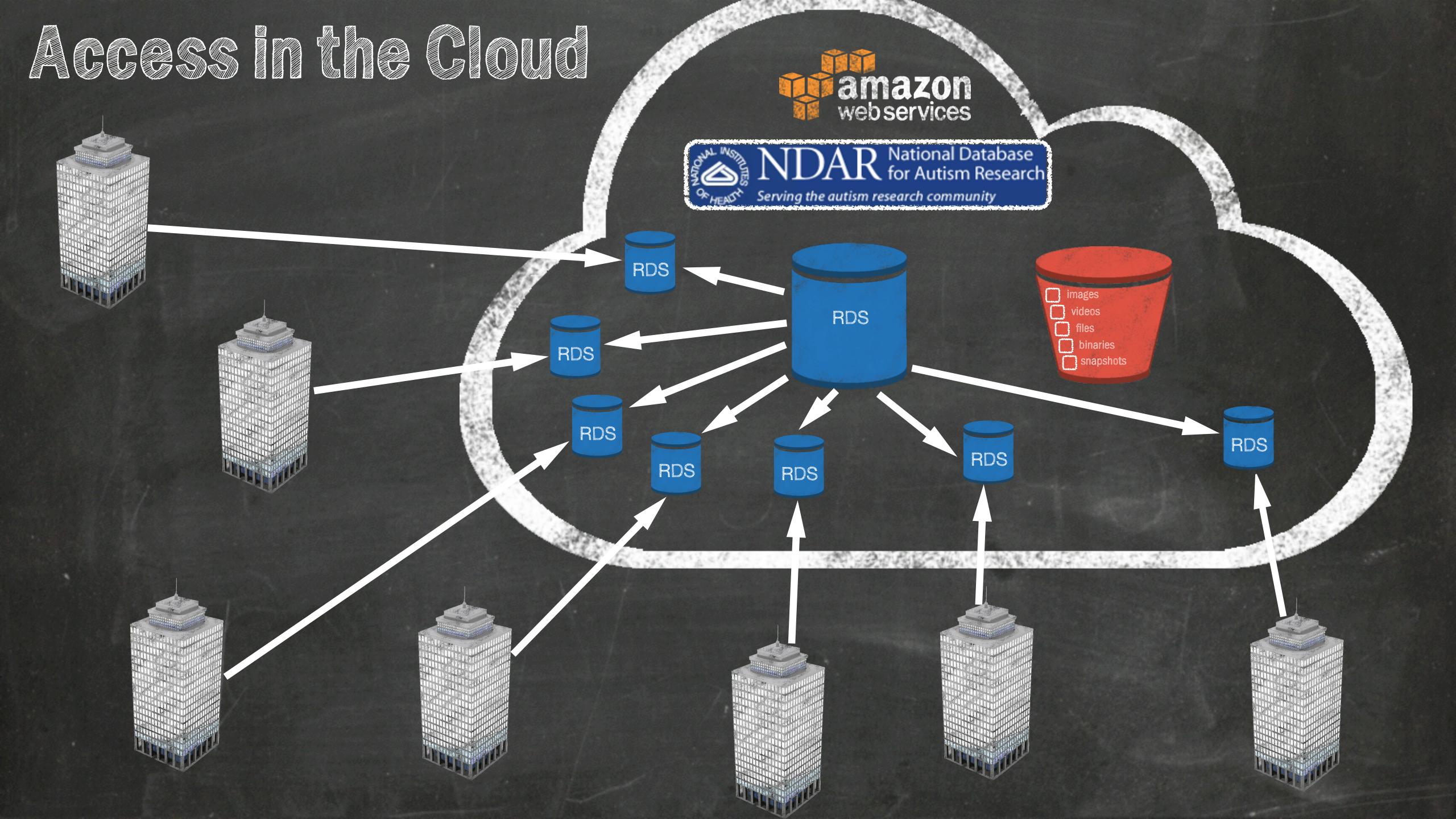


http://ndar.nin.gov/cloud_overview.html

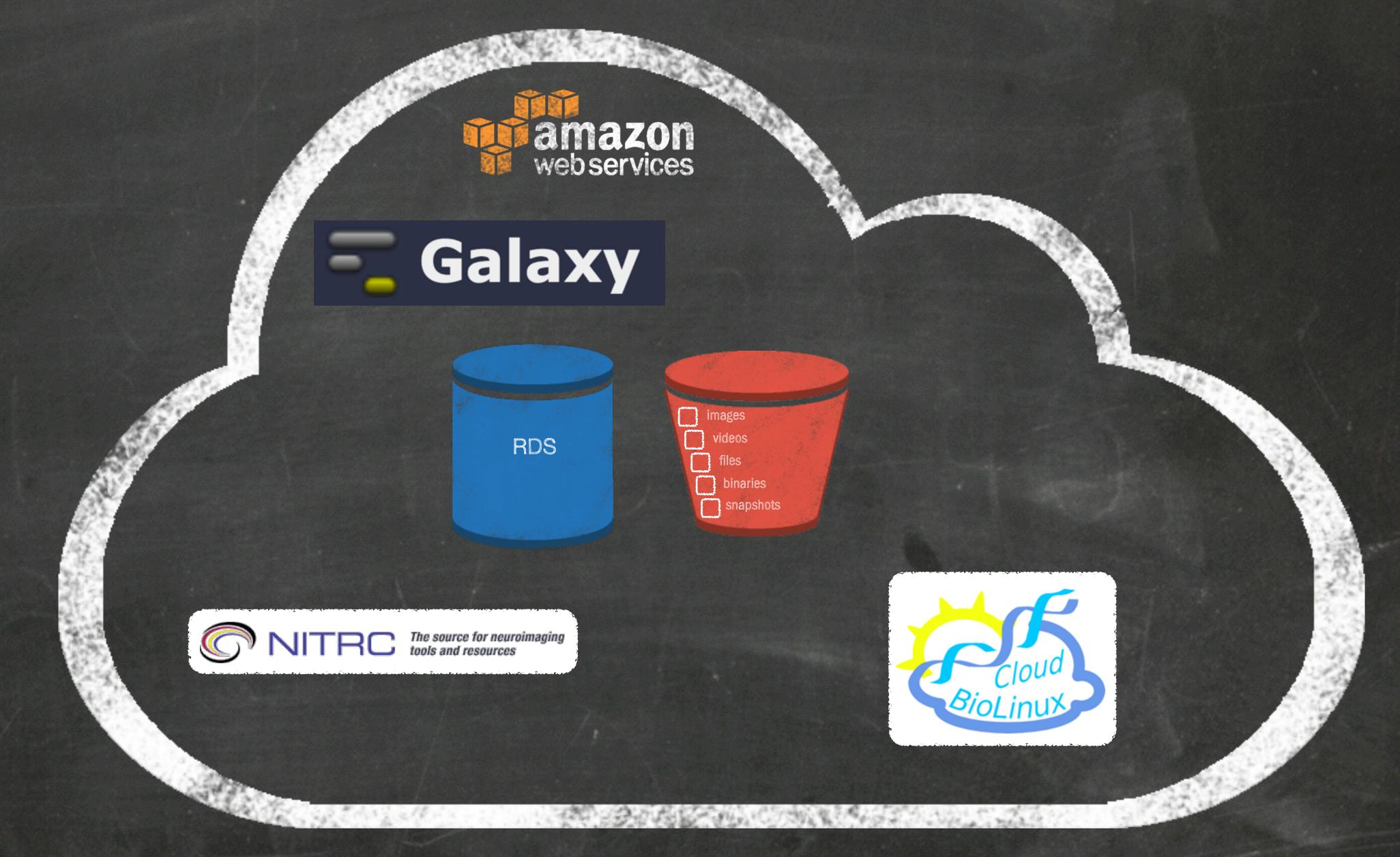
All autism research funded by NIMH must be publicly accessible

NDAR provides a web interface to query the aggregate data set





Gomputation in the Gloud



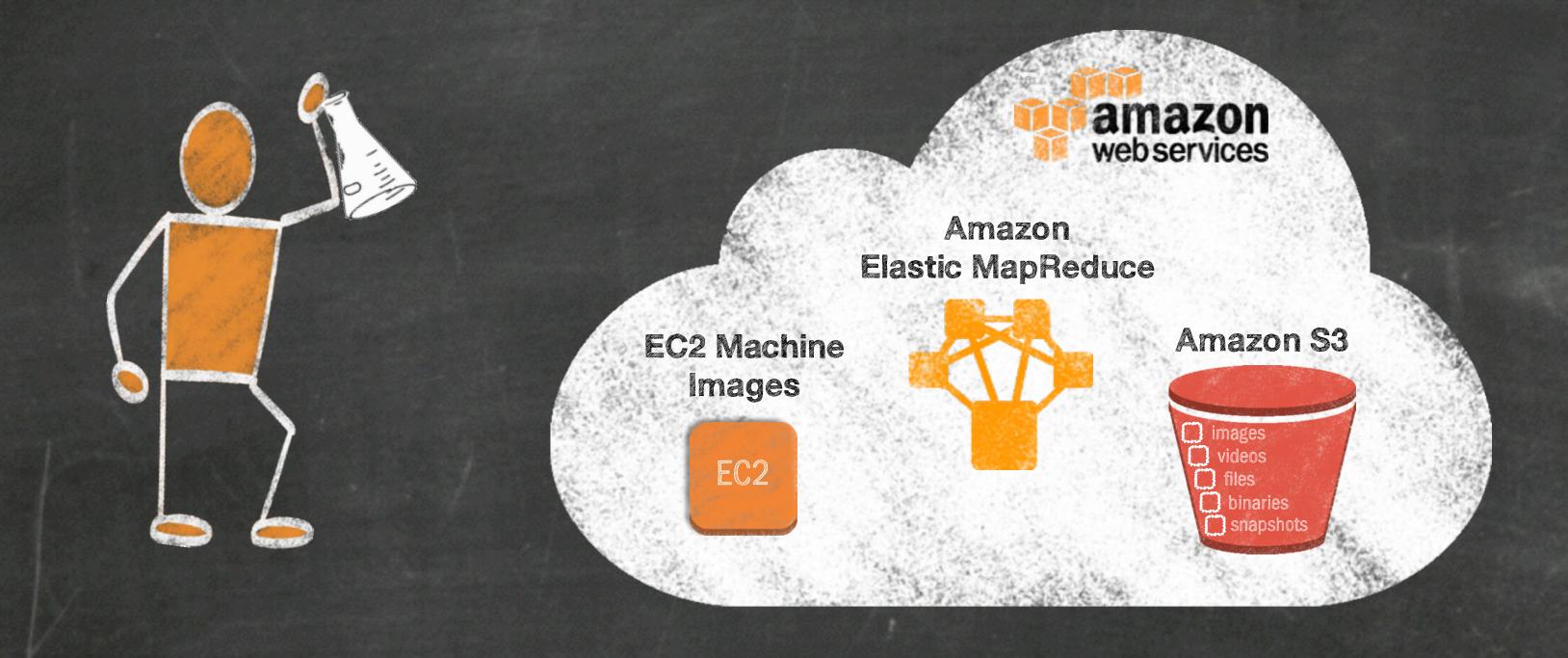
Where is this coins

1. Researcher conducts experiment



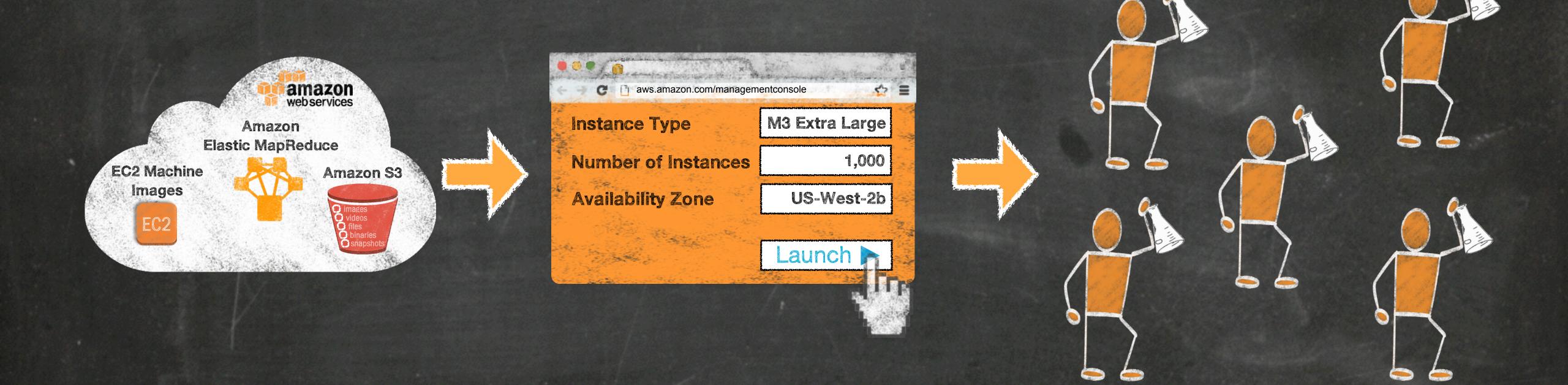
Where is this coins?

- 1. Researcher conducts experiment
- 2. Experimental data and results uploaded to the cloud along with reproducible machine images



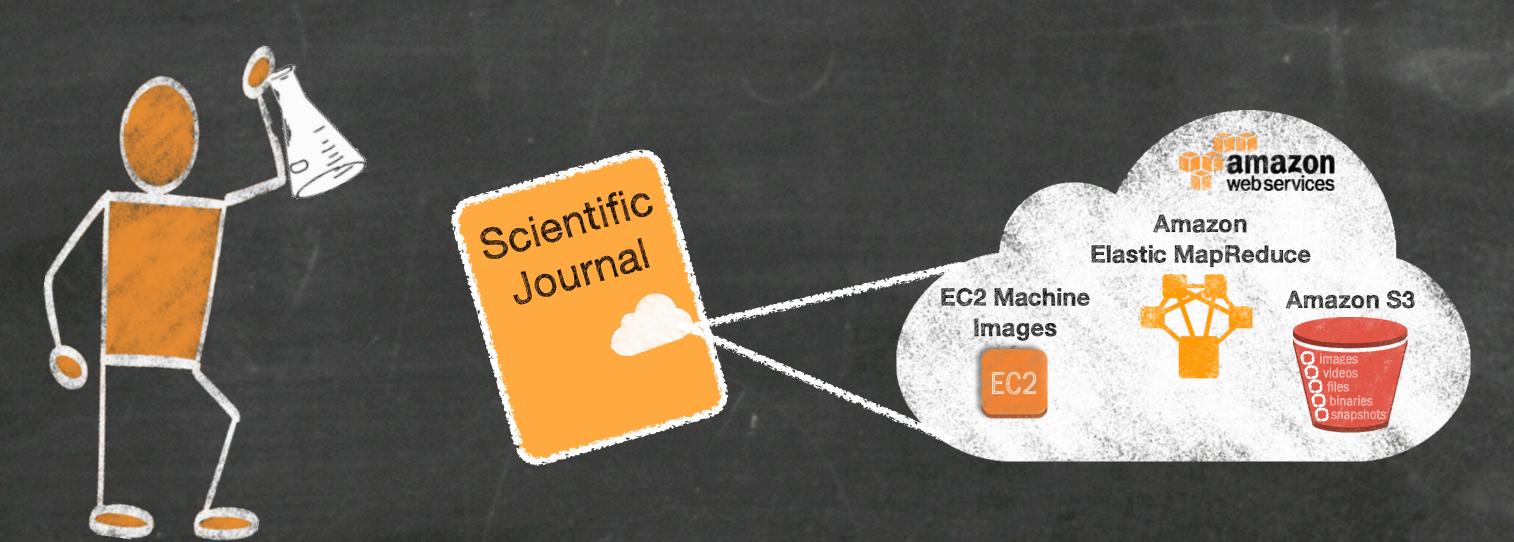
Whele is this coins

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- 3. Reviewers leverage cloud resources to reproduce and validate results.



Whele is this coins

- 1. Researcher conducts experiment
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- 3. Reviewers leverage cloud resources to reproduce and validate results.
- 4. Results published in a peer-reviewed journal, including references (e.g. DOIs) to cloud data and AMIs



Where is this Going?

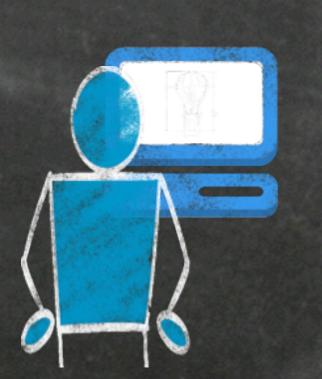
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- 5. Other researchers use these resources as a jumping off point for further research, also publishing their results in the cloud.













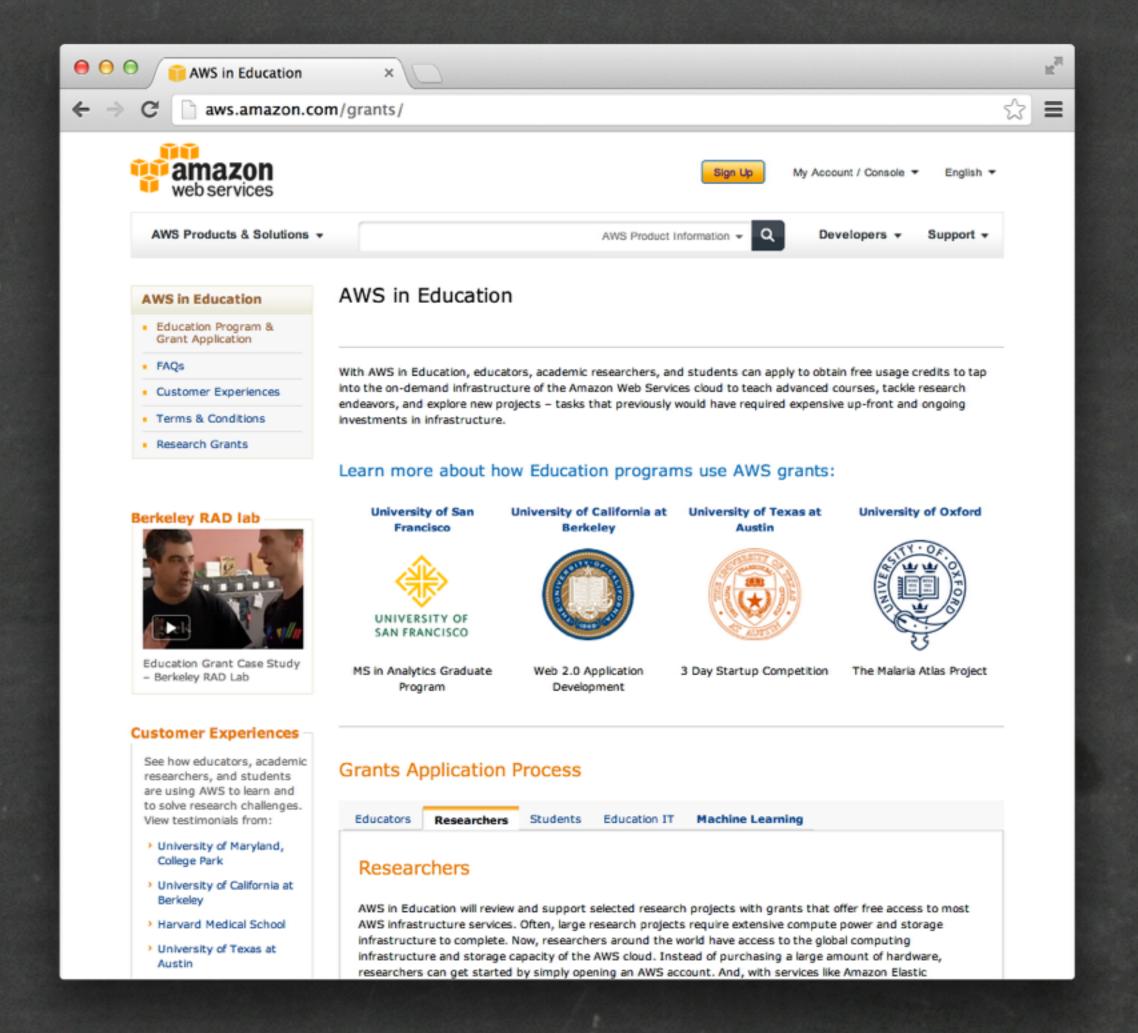
Where is this coins





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- 5. Other researchers use these resources as a jumping off point for further research, also publishing their results in the cloud.
- 6. Automated workflows re-run the original researcher's experiments on the new data using the original machine images. Interesting results trigger notifications and further review.

AWS AGOGEMIC GRANTS



AWS.amazon.com/grants

